

FIELD STUDY REPORT

Enhanced Oxidative Bioremediation of *cis*-Dichloroethene (*cis*-DCE)
and Vinyl Chloride (VC) using Electron Shuttles

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List of Abbreviations and Acronyms

AFB	Air Force Base
AFCEE	Air Force Center for Engineering and the Environment
aq	Aqueous
ASTM	American Society for Testing Materials
AVS	Acid volatile sulfide
Bgs	Below ground surface
BW	Between biowalls
°C	Degrees Celsius
C _{AVS}	Concentration of acid volatile sulfide
C _{DG}	Concentration downgradient of biowall
C _{UG}	Concentration upgradient of biowall
C _{S-2 dissolved}	Concentration of dissolved sulfide
C _{S-2 minerals}	Concentration of non-nanoparticulate sulfide minerals
C _{S-2 nanoparticles}	Concentration of nanoparticulate sulfide minerals
<i>cis</i> -1,2-DCE	<i>cis</i> -1,2-Dichloroethene
cm	Centimeters
cm/sec	Centimeters per second
COC	Contaminant of concern or chain of custody
CrRS	Chromium reducible sulfide
C _{SO4}	Sulfate concentration
CV	Coefficient of variance
δ ¹³ C	Delta carbon 13
DCE	Dichloroethene
DG	Downgradient
DO	Dissolved oxygen
DOC	Dissolved organic carbon
E _h	The oxidation-reduction potential with respect to the reference cell used in the field probe, measured in volts or millivolts (this is the reading measured in the field)
EGME	Ethylene glycol monoethyl ether
EMP	Electron Microprobe
ES	Executive summary
ESTCP	Environmental Security Technology Certification Program
FSP	Field Sampling Plan
f _{abiotic}	Fraction of degradation attributable to abiotic transformation
f _{oc}	Fraction of organic carbon
ft	Feet
ft/day	Feet per day
ft/ft	Feet per foot
ft/yr	Feet per year

List of Abbreviations and Acronyms (cont.)

g	Grams or gaseous
GWERD	Ground Water and Ecosystems Research Division
h ⁻¹	Reciprocal hours
IAP	Ion activity product
IDW	Investigation derived waste
k	Generic rate constant or second-order rate constant
k'	Pseudo first-order rate constant
k ₁	Rate constant for step 1
k ₂	Rate constant for step 2
K _{oc}	Organic carbon partition coefficient
k _{overall}	Overall removal rate constant
K _{sp}	Solubility product constant
L	Liquid
L/d	Liters per day
L/kg	Liters per kilogram
L m ⁻² h ⁻¹	Liters per square meter per hour
L _{SO4}	Volumetric loading rate of sulfate
M	Moles per liter or molar
m ² /g	Square meters per gram
m ² /L	Square meters per liter
MCL	Maximum contaminant level
MEEA	Methane, Ethane, Ethene, and Acetylene
mg/kg	Milligrams per kilogram
mg-S/kg	Milligrams sulfur per kilogram
mg/L	Milligrams per liter
mg L ⁻¹ d ⁻¹	Milligrams per liter per day
mV	Millivolts
µg/L	Micrograms per liter
µm	Micrometers
µM	Micromoles per liter or micromolar
µmol/L	Micromoles per liter or micromolar
N	Number
ND	Not detected
NA	Not applicable or not analyzed
nm	Nanometers
NFESC	Naval Facilities Engineering Service Center
NRMRL	National Risk Management Research Laboratory
ORP	Oxidation-reduction potential
OU	Operable Unit
PCE	Tetrachloroethene
PCR	Polymerase Chain Reaction

List of Abbreviations and Acronyms (cont.)

PHREEQC	Geochemical equilibrium modeling program developed by the United States Geological Survey (pH, REdox, EQuilibrium model written in C programming language)
pH _{zpc}	pH of the zero-point-of-charge
PPE	Personal protective equipment
PVC	Polyvinyl chloride
Q	Volumetric flow rate
QA/QC	Quality assurance/quality control
SHE	Standard hydrogen electrode
SI	Saturation Index
SOP	Standard operating procedure
SS	Spill Site
SSA	Specific surface area
SWMU	Solid waste management unit
TDS	Total dissolved solids
TCE	Trichloroethene
TOC	Total organic carbon
UG	Upgradient
USACE	United States Army Corps of Engineers
USEPA	United States Environmental Protection Agency
USGS	United States Geological Survey
VC	Vinyl chloride
VOA	Volatile organic analysis
VOC	Volatile organic compound
VOC _{DG}	Downgradient VOC concentration
VOC _{UG}	Upgradient VOC concentration
W	Within biowall
WDG	Within upgradient biowall
WUG	Within upgradient biowall
ζ	Hydraulic residence time

Executive Summary

E1 Introduction

Biogeochemical transformation is defined as “processes where contaminants are degraded by abiotic reactions with naturally occurring and biogenically-formed minerals in the subsurface” (AFCEE et al., 2008). These biogenically-formed minerals are created as a result of biogeochemical reactions typically under anaerobic iron- and sulfate-reducing conditions. Biogenically-formed minerals are particularly important because they are continuously replenished in the subsurface and have high surface area and reactivity. *In situ* biogeochemical treatment systems are defined as systems that capitalize and/or enhance such natural processes via engineered reaction zones in the subsurface. Examples of this application include permeable reactive barriers (e.g., biowalls) and injection of organic carbon (e.g., soluble electron donors or vegetable oil emulsions) into a contaminated aquifer with the specific purpose of creating biogenically-formed minerals.

The use of organic carbon-based permeable reactive barriers for treating chlorinated ethenes is an emerging technology that has shown its potential to be a cost-effective method of treatment (AFCEE, 2008). A carbon-based substrate such as plant mulch or vegetable oil is used to promote *in situ* biogeochemical transformation of chlorinated solvents such as trichloroethene (TCE) and tetrachloroethene (PCE) into benign end products such as carbon dioxide, chloride ion, and water. Some of the minerals which have been found to degrade chlorinated solvents such as TCE include the iron monosulfide minerals mackinawite (Butler and Hayes, 1999 and 2001; Jeong and Hayes, 2007) and troilite (Sivavec et al., 1995), the iron disulfide pyrite (Weerasooriya and Dharmasena, 2001; Lee and Batchelor, 2002a), magnetite (Lee and Batchelor, 2002a; Ferrey et al., 2004), green rust phases (Lee and Batchelor 2002b, Christianson and Stipp, 2003; Maithreepala and Doong, 2005), and iron phyllosilicates such as biotite (Lee and Batchelor, 2004). **Table ES-1** presents a summary of these minerals and their characteristics. The minerals include iron sulfides of different iron-sulfur stoichiometries, mixed valence iron green rusts, and other iron oxides and oxyhydroxides. Some of these minerals are naturally occurring and some are formed via biogeochemical processes. Many of these minerals were detected in several biowalls during this study.

As *in situ* biogeochemical treatment systems are still under development and few field-scale systems have been completed, the processes and mechanisms need to be more fully understood before the technology can gain regulatory acceptance and widespread use.

In April 2007 a workshop was facilitated by the NAVFAC Engineering Service Center (NAVFAC ESC), the Air Force Center for Engineering and the Environment (AFCEE), the United States Environmental Protection Agency (USEPA), the Environmental Security Technology Certification Program (ESTCP), and CDM. Approximately thirty (30) experts in the field of biogeochemical transformations from around the country were invited to participate in the workshop. The workshop was conducted in conjunction with related AFCEE training however, attendance was by invitation only. The purpose of the workshop was to discuss the current understanding of *in situ* biogeochemical transformation processes, identify research and demonstration needs, and provide a foundation to develop practical engineering guidance. The

results presented in this report are part of an effort to meet some of the data needs and recommendations suggested by the workshop participants.

The investigation reported herein was not part of the original scope of project ER0316. The original scope of project ER0316 involved demonstration and validation of the use of electron shuttles compounds for the oxidative biodegradation of *cis*-1,2-dichloroethene (*cis*-DCE) and vinyl chloride (VC). However, results from a treatability study using radiolabeled vinyl chloride were not encouraging, therefore the project was cancelled in May 2006. Upon cancellation of ER0316, obligated ESTCP funds were redirected towards two related and parallel efforts. The first effort was a Workshop on *In Situ* Biogeochemical Transformation. A separate report on the findings of this workshop was previously delivered and has been published (AFCEE et al., 2008). The second effort involved sampling and analysis of Air Force biowall sites where biogeochemical transformation appears to have been occurring are reported here.

Table ES-1 Summary of Relevant Iron Phases

Phase	Formula	Composition	Reaction	Notes
Pyrite	FeS ₂	53.4% Fe, 46.6% S	$\text{Fe}^{2+}(\text{aq}) + \text{S}^0(\text{aq}) + \text{S}^{2-}(\text{aq}) \rightarrow \text{FeS}_2(\text{pyrite})$	Precipitation is often kinetically inhibited, usually forms from marcasite.
Marcasite	FeS ₂	53.4% Fe, 46.6% S	$\text{Fe}^{2+}(\text{aq}) + \text{S}^0(\text{aq}) + \text{S}^{2-}(\text{aq}) \rightarrow \text{FeS}_2(\text{marcasite})$	Intermediate phase in the conversion of pyrrhotite to pyrite. Generally unstable.
Greigite	$\text{Fe}^{+2}\text{Fe}^{+3}_2\text{S}_4$	56.6% Fe, 43.4% S	$\text{Fe}^{2+}(\text{aq}) + 2\text{Fe}^{3+}(\text{aq}) + 4\text{S}^{2-}(\text{aq}) \rightarrow \text{Fe}_3\text{S}_4(\text{greigite})$	Does not precipitate directly, generally formed from pyrrhotite, tends to be unstable, and converts to marcasite. Contains both ferrous and ferric iron.
Pyrrhotite	Fe _{1-x} S	59.1-63.5% Fe, 36.5-40.9% S	$\text{Fe}^{2+}(\text{aq}) + \text{S}^{2-}_{1-x}(\text{aq}) \rightarrow \text{FeS}_{1-x}(\text{pyrrhotite})$	Iron sulfide in which ferrous iron vacancies are charge balanced by ferric iron in the structure.
Troilite	FeS	63.5% Fe, 36.5% S	$\text{Fe}^{2+}(\text{aq}) + \text{S}^{2-}(\text{aq}) \rightarrow \text{FeS}(\text{troilite})$	Pyrrhotite without vacancies. Often referred to as “stoichiometric pyrrhotite”
Mackinawite	FeS _{1-x}	>63.5% Fe, <36.5% S	$\text{Fe}^{2+}(\text{aq}) + \text{S}^{2-}(\text{aq}) \rightarrow \text{FeS}(\text{mackinawite})$	Thought to be the first phase formed from solution, most iron rich (sulfur poor) phase.
Ferrous Hydroxide	Fe(OH) ₂	62.9% Fe, 36.0% O	$\text{Fe}^{+2} + 2\text{H}_2\text{O} \rightarrow \text{Fe}(\text{OH})_2(\text{s}) + 2\text{H}^+$	Ferrous end member of the green rust series. Occurs under iron-reducing conditions.
Ferrous Oxide	FeO	77.7% Fe, 22.3% O	$\text{Fe}^{+2} + \text{H}_2\text{O} \rightarrow \text{FeO}(\text{s}) + 2\text{H}^+$	Not known to precipitate directly from solution.
Hydroxycarbonate Green Rust	$\text{Fe}^{+2}_4\text{Fe}^{+3}_2(\text{OH})_{12}[\text{CO}_3]$	54.5% Fe, 41.6% O, 2.0% C	$6\text{Fe}^{+2} + \text{CO}_3^{-2} + 12\text{H}_2\text{O} \rightarrow [\text{Fe}^{+2}_4\text{Fe}^{+3}_2(\text{OH})_{12}][\text{CO}_3](\text{s}) + 12\text{H}^+ + 2\text{e}^-$	Mixed ferrous/ferric iron phases with a crystalline platy habit. Form under mildly reducing conditions. Unstable in the presence of atmospheric oxygen.
Hydroxysulfate Green Rust	$\text{Fe}^{+2}_4\text{Fe}^{+3}_2(\text{OH})_{12}[\text{SO}_4]$	52.8% Fe, 40.3% O, 5.0% S	$6\text{Fe}^{+2} + \text{SO}_4^{-2} + 12\text{H}_2\text{O} \rightarrow [\text{Fe}^{+2}_4\text{Fe}^{+3}_2(\text{OH})_{12}][\text{SO}_4](\text{s}) + 12\text{H}^+ + 2\text{e}^-$	
Hydroxychloride Green Rust	$\text{Fe}^{+2}_2\text{Fe}^{+3}(\text{OH})_8[\text{Cl}]$	49.4% Fe, 37.8% O, 10.5% Cl	$4\text{Fe}^{+2} + \text{Cl}^- + 8\text{H}_2\text{O} \rightarrow [\text{Fe}^{+2}_3\text{Fe}^{+3}(\text{OH})_8][\text{Cl}](\text{s}) + 8\text{H}^+ + \text{e}^-$	
Hydroxy Green Rust	$\text{Fe}^{+2}_2\text{Fe}^{+3}(\text{OH})_7$	58.5% Fe, 39.1% O	$3\text{Fe}^{+2} + 7\text{H}_2\text{O} \rightarrow [\text{Fe}^{+2}_2\text{Fe}^{+3}(\text{OH})_7](\text{s}) + 7\text{H}^+ + \text{e}^-$	
Hydroxy Green Rust	$\text{Fe}^{+2}\text{Fe}^{+3}(\text{OH})_5$	56.8% Fe, 40.7% O	$2\text{Fe}^{+2} + 5\text{H}_2\text{O} \rightarrow [\text{Fe}^{+2}\text{Fe}^{+3}(\text{OH})_5](\text{s}) + 5\text{H}^+ + \text{e}^-$	
Hydroxy Green Rust	$\text{Fe}^{+2}_2\text{Fe}^{+3}(\text{OH})_7$	58.5% Fe, 39.1% O	$3\text{Fe}^{+2} + 8\text{H}_2\text{O} \rightarrow [\text{Fe}^{+2}_2\text{Fe}^{+3}(\text{OH})_7](\text{s}) + 8\text{H}^+ + 2\text{e}^-$	Exists both as a primary crystalline mineral and a secondary (sedimentary) form.
Magnetite	Fe ₃ O ₄	72.4% Fe, 27.6% O	$3\text{Fe}^{+2} + 4\text{H}_2\text{O} \rightarrow \text{Fe}_3\text{O}_4 + 8\text{H}^+ + 2\text{e}^-$	
Lepidocrocite	γ-FeOOH	62.9% Fe, 36.0% O	$\text{Fe}^{+2} + 2\text{H}_2\text{O} \rightarrow \gamma\text{-FeOOH} + 3\text{H}^+ + \text{e}^-$	
Hematite	Fe ₂ O ₃	69.9% Fe, 30.1% O	$2\text{Fe}^{+2} + 3\text{H}_2\text{O} \rightarrow \text{Fe}_2\text{O}_3 + 6\text{H}^+ + 2\text{e}^-$	
Ilmenite	FeTiO ₃	36.8% Fe, 31.6% Ti, 31.6% O	$\text{Fe}^{+2}(\text{aq}) + \text{Ti}^{+4}(\text{aq}) + 3\text{H}_2\text{O} \rightarrow \text{FeTiO}_3(\text{s}) + 6\text{H}^+(\text{aq})$	

E1.1 Objectives of Study

The objectives of the investigation for which results are presented in this report, included:

- Evaluate methods to investigate the iron and sulfide mineralogy of the *in situ* biogeochemical treatment systems and subsurface soil materials.
- Perform and evaluate the utility of these methods to improve the understanding of biogeochemical reduction, including differences between abiotic processes and biotic reductive dechlorination.
- Determine the conditions under which the potential for formation of appropriate forms of iron sulfides and biogeochemical reduction of chlorinated solvents is optimal.
- Investigate and recommend analytical procedures to evaluate degradation of chlorinated solvents by biogeochemical transformation.
- Use the information gained from this investigation to develop practical guidelines for designing and optimizing substrate amendments (e.g., iron or sulfate) to stimulate biogeochemical reduction for differing geochemical and hydrogeologic conditions.

E1.2 Approach

In this investigation, existing treatment systems where biogeochemical transformation processes may be occurring or is purposefully targeted were evaluated using a combination of standard (i.e., methods commonly used in environmental investigations) and nonstandard analyses and techniques (i.e., analyses used mainly for research). The treatment systems that were evaluated included:

- The Operable Unit 1 (OU-1) and Spill Site 17 (SS-17) mulch biowalls at Altus AFB, Oklahoma.
- A laboratory column study that was constructed using materials from the Altus AFB SS-17 biowall.
- The WP-14 mulch biowall at Dover AFB, Delaware.
- The Ash Landfill mulch biowalls at Seneca Army Depot Activity, New York.
- An emulsified vegetable oil pilot test at the Solid Waste Management Unit 97 (SWMU-97) Site, Dugway Proving Ground, Utah.

Table ES-2 presents a summary of the design and operating details associated with each of these systems. The Altus AFB, Dover AFB, and Seneca Army Depot Activity study sites were mulch-containing biowalls whereas the Dugway Proving Ground study site was an emulsified vegetable oil bioremediation area. The Altus AFB and Dover AFB walls included different biowall compositions in different portions of each biowall (see **Table ES-2**) and samples were collected from each location. In addition, a laboratory column (i.e., USEPA column) was studied. This column was designed and operated similarly to the Altus AFB SS-17 biowall but hematite was added to the mulch mixture.

Table ES-2 - Summary of System Design Parameters and Background Information for Each Site

Location	Installation Date	Dimensions	Biowall Composition ^a	Residence Time (days)	Historic VOC Concentrations (µg/L) ^b	Background Geochemistry ^c
Altus AFB (OU-1 site), Oklahoma	July 2002 (pilot)	455 feet long by 24 feet deep by 1.5 feet wide	Tree mulch (48%), cotton gin compost (10%), river sand (42%)	9-13.7	TCE: 8,000 DCE: 1,800 VC: Non-detect prior to installation	DO: 0 to 2 mg/L ORP: 0 to +150 mV Sulfate: 1,500 to 2,000 mg/L
Altus AFB (SS-17 site), Oklahoma	March-May 2005 (full-scale)	5,400 feet wide by 35 feet deep by 2 feet wide.	Tree mulch (42%), cotton gin trash (11%), concrete sand (32%), 0.75 in. gravel (15%)	1-50	TCE: 31,800 DCE: 6,400 VC: 11,600	DO: 0 to 2 mg/L ORP: 0 to +150 mV Sulfate: 1,500 to 2,000 mg/L
USEPA Column	2005	15 cm diameter by 46 cm length	Altus AFB SS-17 mixture plus 36% sand and 4% hematite.	17	TCE: 2,000	Sulfate: 1,500 to 2,000 mg/L
Dover AFB (WP-14 site), Delaware North Transect	December-04	Dual Wall 250 feet long by 25 feet deep by 2 feet wide	Tree mulch (50%), silty river sand (45%), and limestone (5%)	130 (UG wall), 195-391 (DG wall)	PCE: 3,400 TCE: 930 DCE: 2,000 VC: 63 µg/L	DO: 1 to 5 mg/L ORP: +200 to +400 mV Sulfate: <25 mg/L
Dover AFB (WP-14 site), Delaware South Transect	December-04	Dual Wall 250 feet long by 25 feet deep by 2 feet wide	Tree mulch (50%), silty river sand (40%), limestone (5%), and gypsum (5%)	130 (UG wall), 195-391 (DG wall)	PCE: 3,400 TCE: 930 DCE: 2,000 VC: 63 µg/L	DO: 1 to 5 mg/L ORP: +200 to +400 mV Sulfate: <25 mg/L
Seneca Army Depot Activity (Ash Landfill site), New York	October-06 (full-scale)	Single Double-Wide and Dual Biowall System. 1,500 linear feet, 10 to 15 feet deep by 3.0 to 6.0 feet wide	Mulch (50%) and Sand (50%). Mulch (6,240 cubic yards) in upgradient biowall coated with 15,600 gallons of vegetable oil	16-66	TCE: 2,000 DCE: 960 VC: 95	DO: 2 to 4 mg/L ORP: 0 to 100 mV Sulfate: 500 to 900 mg/L

Table ES-2 - Summary of System Design Parameters and Background Information for Each Site (cont.)

Location	Installation Date	Dimensions	Biowall Composition ^a	Residence Time (Days)	Historic VOC Concentrations (µg/L) ^b	Background Geochemistry ^c
Dugway Proving Ground (SWMU-97 site), Utah	November-04 (pilot)	Four Injection Wells on 10-foot centers	Direct Injection of Field Mixed Emulsion - approximately 3000 lbs. vegetable oil mixed with lecithin, sodium bromide, and site groundwater	NA	TCE: 2,300 DCE: <1.0 VC: Non-Detect	DO: <1.5 mg/L ORP: <0 mV Sulfate: 10,470 mg/L

Notes:

a) By volume.

b) Contaminants are maximum concentrations prior to treatment or upgradient of treatment zone in micrograms per liter (µg/L).

c) Background geochemistry for dissolved oxygen (DO) and sulfate is an average or range of concentrations in milligrams per liter (mg/L), or in millivolts (mV) for oxidation-reduction potential (ORP).

UG - upgradient.

DG - downgradient.

These sites were selected because they varied with respect to biowall composition, organic substrate addition, groundwater composition, hydrogeologic considerations, and chlorinated ethene transformation. Thus they provided a good opportunity to study the effects of these differences on biogeochemical transformation processes.

The approach to this effort followed the three basic lines of investigation proposed by Brown et al. (2007), which are as follows:

- Abiotic footprints
- Plume degradation patterns
- Mineralogical characterization

In addition, a few new approaches, such as the use of the electron microprobe (EMP) were used.

The concept of abiotic footprints is that the abiotic degradation pathway leads to a different set of end products through a different set of intermediary compounds when compared to biotic transformations. The analysis of abiotic footprints involves comparison of parameters associated with strictly abiotic transformation to those associated with biological transformation processes. Buildup of daughter products is characteristic of biological transformation of PCE and TCE. In the case where the chlorinated solvents are rapidly transformed to carbon dioxide and water via unstable intermediates, the concentrations of all compounds decrease with distance (i.e., there is no build-up of daughter products). Such a plume pattern is characteristic of abiotic transformation.

Mineralogical characterization is important for making the link between the most effective systems and the mineralogy of that system. Characterization included not only the identification of the reduced iron phases present in the substrate (i.e., organic carbon source), but also the degree of crystallinity, quantity, grain size, associations, and morphology (i.e., form), all of which may contribute to system performance. Surface is also important, but is difficult to measure directly in complex aquifer sediments and must be estimated from geometry and particle size distribution. The mineralogical characterization was conducted using unconventional analytical techniques, such as the electron microprobe.

In addition to the basic lines of investigation described above, the inorganic geochemical processes that are occurring within the systems were investigated using chemical equilibrium computer modeling. The modeling helped to understand the inorganic chemical reactions occurring within the treatment zones and the upgradient and downgradient groundwater.

E2 Sampling and Analysis

E2.1 Samples Collected

Groundwater samples were collected from upgradient, downgradient and reaction-zone well locations (i.e., either within the biowall or vegetable oil injection zone). Biowall mulch or injection zone aquifer matrix samples were collected from several locations and depths at each site and preserved. Samples were also collected from the USEPA columns.

E2.2 Analyses Performed

The following analyses were performed on the biowall mulch, column mulch, and reactive zone soil:

- Total organic carbon, total inorganic carbon, total carbon, and moisture content.
- Electron microprobe analyses.
- Acid volatile sulfides (AVS), chromium-reducible sulfides (CrRS), sulfate, and total sulfur.
- Iron extractions (dithionite, ascorbate, 0.5 M HCl, and HNO₃ digestion).
- The following analyses were performed on the USEPA column influent/effluent samples and field site upgradient, downgradient, and in wall groundwater samples:
 - General parameters (pH, oxidation-reduction potential, dissolved oxygen, specific conductivity, temperature, ferrous iron, manganese, sulfide, alkalinity, total dissolved solids, and total organic carbon).
 - Anions (chloride, sulfate, sulfide, phosphate, nitrate, nitrite, and fluoride) and cations (sodium, potassium, calcium, magnesium, manganese, and iron).
 - Volatile organic compounds (PCE, TCE, *cis*-1,2-dichloroethene [*cis*-1,2-DCE], and vinyl chloride [VC]).
 - Methane, ethene, ethane, and acetylene.
 - Carbon stable isotopes.

E2.3 Data Analysis

The data were evaluated using the following:

- PHREEQC, a geochemical model for pH, REdox, EQUilibrium model written in C programming language, Parkhurst and Appelo, 1999) identified the reduced iron phase(s) at saturation in the system as well as identifying if sulfate sources are present within the upgradient aquifer.
- Trilinear diagrams (provided general water type and the differences among the upgradient, down gradient, and in-wall samples).
- Statistical analyses such as the mean, median, standard deviation and coefficient of variance (identified variability in the data and provided a convenient means of comparing sample values from one site to those of another).
- VOC and methane, ethene, ethane, acetylene trend plots along the axis of the groundwater plume (used to determine biotic versus abiotic transformation characteristics).

E3 Results and Discussion

A summary of the significant results from this study is presented in this section. Additional results are presented in the full report.

E3.1 Reduced Iron Phase Mineralogy

E3.1.1 Electron Microprobe

Figures ES-1 through **ES-6** are electron microprobe photomicrographs of typical mineral phases identified in samples from the different sites. These photomicrographs illustrate morphology and chemical composition of mineral and non-mineral particles. Iron and other minerals are depicted in lighter shades and carbonaceous materials are depicted in darker shades. **Figure ES-1** shows high surface area framboidal (i.e., spherical clusters of mineral particles – typically pyrite) iron sulfide¹ that was observed in a sample from the Altus AFB OU-1 biowall. This iron sulfide is stoichiometrically similar to iron disulfide and could be pyrite or marcasite. These framboidal phases were frequently observed in samples from the OU-1 biowall. They were not observed in the Altus AFB SS-17 biowall, possibly because concentrations were less than the detection limits (e.g., > 200 mg/kg) for electron microprobe analysis. **Figure ES-2** depicts small non-framboidal iron sulfide grains in a sample from the Altus AFB OU-1 biowall. These grains are associated with organic carbon present in the sample. The forms of iron sulfide present in **Figures ES-1** and **ES-2** have high surface area which can contribute to reactivity towards chlorinated ethenes.

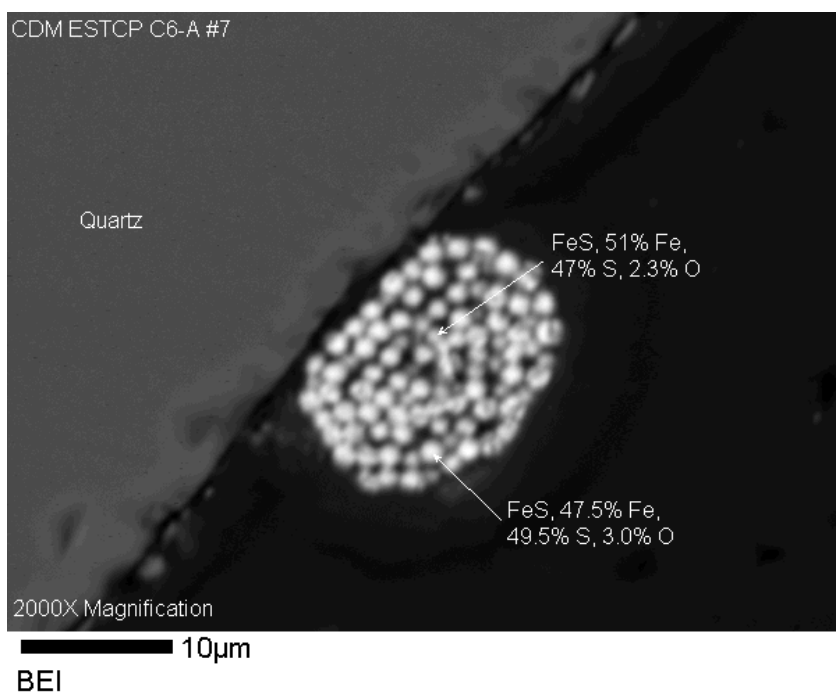


Figure ES-1 - Framboidal Iron Sulfide Grains in Altus AFB OU-1 Sample. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

¹ The term “iron sulfide” used in this document generically references the various minerals containing iron and sulfur and is not intended to imply iron monosulfide specifically.

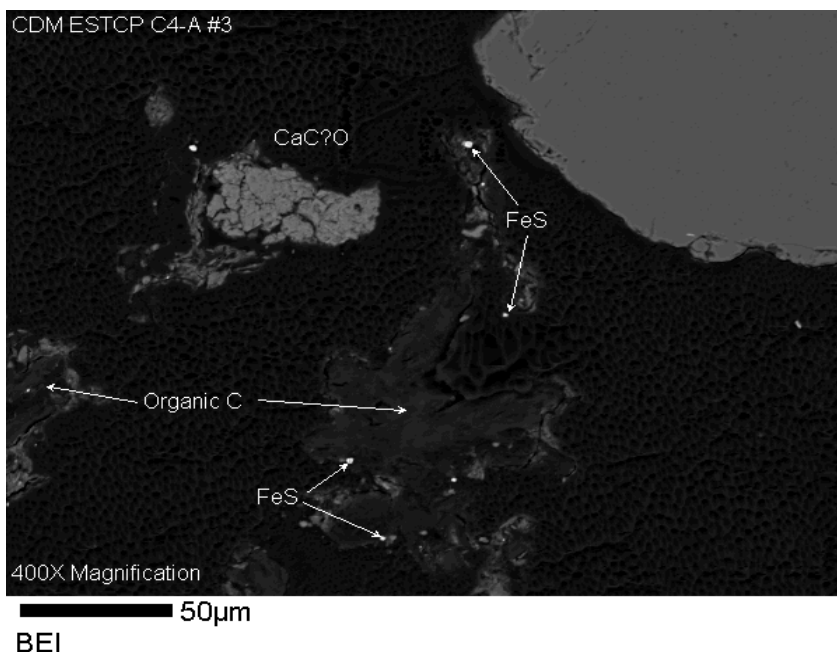


Figure ES-2 - Pyrite Grains Associated with Organic Carbon in Altus AFB OU-1 Sample. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry

Figure ES-3 illustrates a grain of magnetite present in a sample from the Altus AFB SS-17 biowall. While iron sulfide grains were not observed in samples from this biowall, a laboratory column prepared using this material at the USEPA laboratory in Ada, Oklahoma contained framboidal iron sulfides as shown in **Figure ES-4** and **ES-5**. This column was prepared using the Altus AFB SS-17 biowall formulation plus granular hematite. Comparison of **Figure ES-5a** (a backscatter image showing both iron sulfides and iron oxides) and **ES-5b** (a sulfur-specific “dot map” for the same particle shown in **Figure ES-5a**) indicates that an iron sulfide coating is present on an iron oxide grain. Electron microprobe analysis indicated that the iron sulfide coating is on magnetite and not on hematite that was added to the mulch mixture. A framboidal iron sulfide grain is also shown in **Figure ES-5**. These photomicrographs indicate dissolution of magnetite and ilmenite which was common in all of the samples, suggesting that these phases may provide an important source of ferrous iron for iron sulfide precipitation when conditions are favorable (i.e., high rates of sulfate reduction). The USEPA column samples illustrate that iron oxide minerals such as magnetite (at pH < 8.5) and hematite (at pH < 6.7) can provide surface sites for the formation of iron sulfides. Therefore, the addition of specific iron oxides to the mulch should have a beneficial effect as an increase in reactive iron oxides should result in increased biogeochemical transformation.

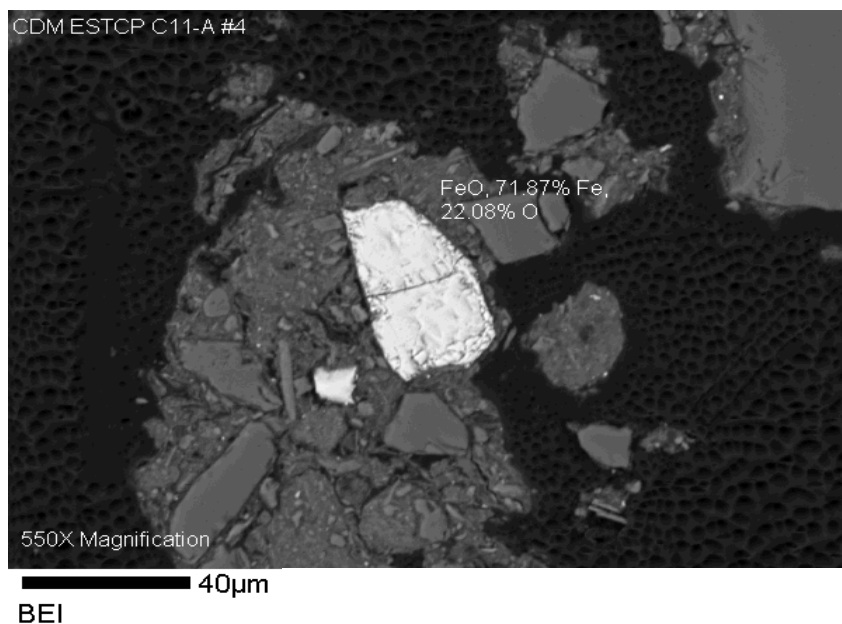


Figure ES-3 - Crystalline Magnetite in Altus AFB SS-17 Sample. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

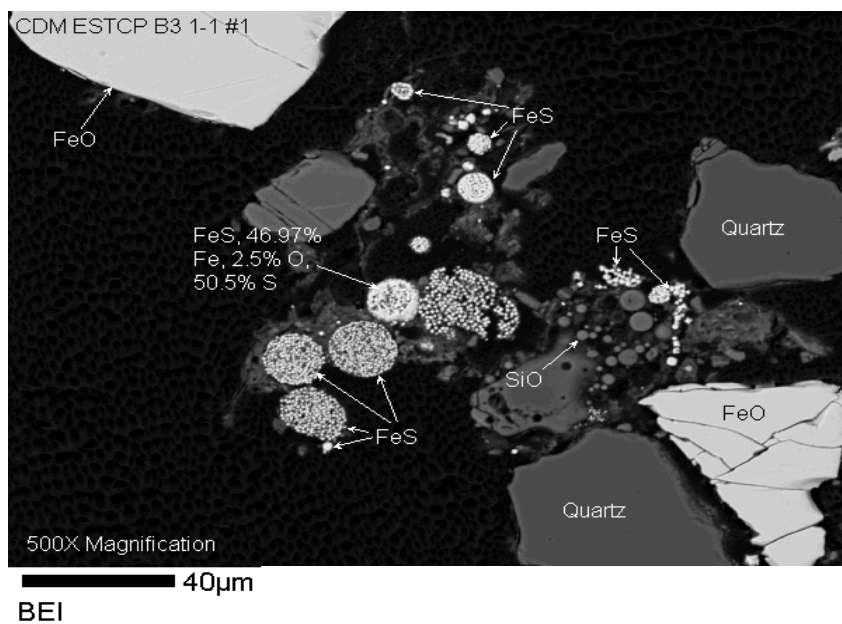
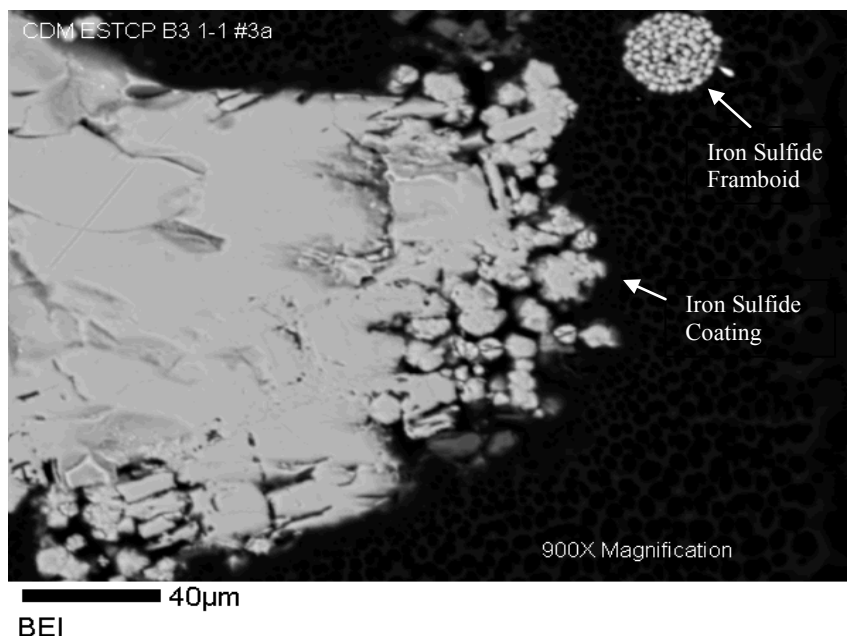


Figure ES-4 - SS-17 Column Showing Framboidal Forms of Iron Sulfide. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry

A



B

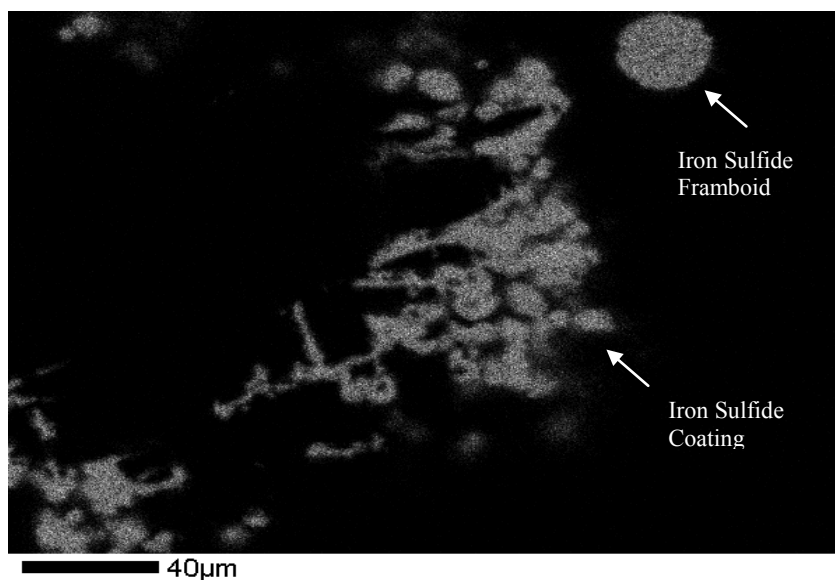


Figure ES-5 - Iron Sulfides Associated with Magnetite and an Iron Sulfide Framboid in an Altus AFB SS-17 Column Sample. Photomicrograph A is a backscatter image showing both iron sulfides and iron oxides. Photomicrograph B shows sulfur only. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

Figure ES-6 is a photomicrograph of a sample collected from the Dover AFB site. Iron sulfides were detected by electron microprobe analysis in the Dover AFB samples but partial oxidation was apparent indicating the iron sulfide was not freshly formed. The grain is also relatively large, and for a given mass of particles, larger particles will have less surface area and reactivity, because of a relatively low ratio of surface area-to-volume. Iron sulfides were not observed in samples from the Seneca Army Depot Activity or Dugway Proving Ground Sites.

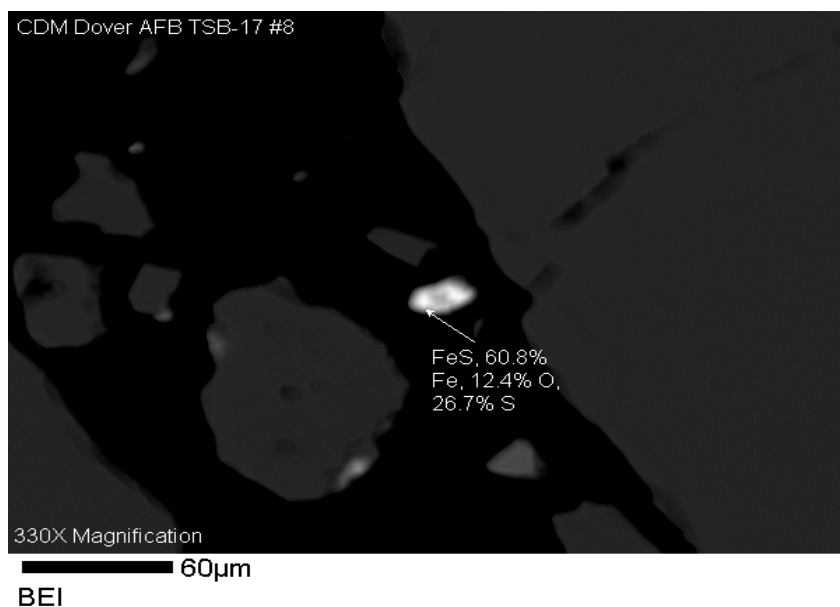


Figure ES-6 - Partially Oxidized Iron Sulfide Grain in Dover AFB Sample. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

Table ES-3 presents a summary of reduced iron phases observed in the samples using electron microprobe as described above. The iron phases that were detected included iron minerals such as magnetite and hematite and various iron sulfides. The data also indicated that several iron sulfides were partially oxidized. Green rusts were not identified conclusively during the investigation. These data indicate that the electron microprobe was a useful tool for identifying specific iron oxides and iron sulfides.

Table ES-3 - Summary of Soil Results for Each Site

Site	Iron Phases Detected (EMP)	Iron Phases Predicted by PHREEQC			Chemical Extractions	
		Under Saturation	At Saturation	Super-Saturation	Median AVS (mg-S/kg)	Median CrRS (mg-S/kg) ^a
Altus AFB OU-1	FeS ₂ , crystalline magnetite	Magnetite	Troilite and mackinawite	Marcasite and pyrite	226	285
Altus AFB SS-17	Crystalline magnetite	Mackinawite and magnetite	Troilite	Marcasite and pyrite	174	23
USEPA Column	FeS ₂ associated with crystalline magnetite and hematite	Magnetite and hematite	Poorly ordered Mackinawite	Marcasite, pyrite, and troilite	1450	1518
Dover AFB North Transect	Partially to completely oxidized FeS and FeS ₂	Magnetite	Poorly ordered mackinawite and crystalline mackinawite	Marcasite, pyrite, and troilite	441	218
Dover AFB South Transect	Partially to completely oxidized FeS and FeS ₂	Magnetite	Poorly ordered mackinawite and crystalline mackinawite	Marcasite, pyrite, and troilite	1414	1453
Seneca Army Depot Activity A	Crystalline and amorphous magnetite	Magnetite	Greigite, poorly ordered mackinawite, and alkaline mackinawite	Marcasite, pyrite, and troilite	64	181
Seneca Army Depot Activity B	Crystalline and amorphous magnetite	Magnetite	Greigite, poorly ordered mackinawite, and alkaline mackinawite	Marcasite, pyrite, and troilite	18	197
Dugway Proving Ground	Ti-bearing hematite or ferrous hydroxide, and ilmenite (some reacted)	Magnetite	Poorly ordered mackinawite and crystalline mackinawite	Marcasite, pyrite, and troilite	80	43

Notes:
a) Reported CrRS values do not include AVS fraction.
EMP - electron microprobe.
PHREEQC - geochemical model (see text for description Section 2.4).

E3.1.2 Geochemical Modeling

Geochemical modeling was also conducted using the model PHREEQC. The model was used to predict which mineral phases were undersaturated, at saturation, and supersaturated.

Undersaturated phases tend to go into solution, supersaturated phases tend to precipitate out of solution, and saturated phases are generally in equilibrium. This model is an equilibrium model and indicates which minerals can be expected to form in solution (i.e., the saturated and supersaturated phases), but does not account for any kinetic limitations to their formation. As illustrated in **Table ES-3**, the modeling indicated that in general, iron oxides (e.g., magnetite and hematite) were undersaturated and thus could be expected to dissolve, and that iron sulfides (e.g., mackinawite, marcasite, troilite, greigite, and pyrite) were generally saturated or supersaturated and thus could be anticipated to form solid precipitates. Geochemical modeling provided an increased understanding of the potential to form specific reactive minerals and how these minerals would form at a given site. This understanding is important with respect to being able to design *in situ* biogeochemical transformation treatment systems because the specific mineral type and form directly control the rate of contaminant destruction.

ES3.1.3 Bulk Chemical Extractions

Bulk chemical extractions of the solid-phase samples were conducted in addition to electron microprobe analysis and geochemical modeling and the results are presented in **Table ES-3**. The concentration of AVS was used to estimate the concentrations of iron monosulfides in the samples and the difference between the concentration of CrRS and AVS was used to estimate concentrations of iron disulfides in the samples. These extractions are operationally defined; the AVS extraction is relatively weaker than the CrRS extraction, and AVS is generally assumed to extract only iron monosulfide and greigite, while CrRS extracts iron mono- and di-sulfides as well as greigite and native sulfur. The data show that the samples from Altus AFB, the USEPA column, and Dover AFB had high concentrations of the iron sulfides and the Seneca Army Depot Activity and Dugway Proving Ground samples had relatively low concentrations. The relative concentrations of total iron sulfides estimated by chemical extraction are generally consistent with the electron microprobe analysis results based on an estimated electron microprobe detection limit of about 200 mg/kg.

ES3.1.4 Mineral Reactivity and Chlorinated Ethene Transformation

The reaction between chlorinated ethenes and iron sulfide phases is believed to occur by the adsorption of the chlorinated ethene onto a finite number of reactive sites on the surfaces of the mineral, followed by reductive dechlorination and deactivation or loss of reactivity of the site (Lee and Batchelor, 2002a). Therefore, the rates for the abiotic degradation of chlorinated ethenes are dependent on the surface area of the reactive minerals. Rate constants for a given mineral can vary by orders of magnitude depending on the grain size of the particles, the total concentration present, and the surface area. The overall order of the surface area-normalized reaction rate constants for the common reduced iron phases is typically reported as follows (Lee and Batchelor, 2002a; Lee and Batchelor, 2002b; Butler and Hayes, 1999 and Butler and Hayes, 2001):

Mackinawite > Green Rusts > Pyrite >> Magnetite

However, a wide range of rate constants have been reported for various iron minerals. Different methods of preparation (e.g., freeze drying, preparation under anoxic conditions) and surface area measurement are possible explanations for the differences. Nevertheless, the data suggest that the specific reactivity of pyrite may in fact have similar reactivity than iron monosulfide for a constant surface area. Thus the universe of iron sulfides responsible for *in situ* biogeochemical transformation of chlorinated ethenes appears to be broader than iron *monosulfide*.

Another important factor in maximizing the rate of reaction between chlorinated ethenes and iron sulfides is the surface area of the iron sulfides. While adjusting the pH from 6 to 8 can increase the rate constant by a factor of 5 (all other variables remaining constant), a decrease in the median grain size of the iron sulfide particles from 1 μm to 10 nm can increase the rate constant by 100 times. Although nanoparticles were not likely present in any of the field systems investigated in this study, several investigators have reported the production of nanoparticulate iron monosulfides by sulfate-reducing bacteria (Ohfuji and Rickard, 2006).

In general, to produce small diameter iron sulfide particles (such as framboidal pyrite), the nucleation rate must be very rapid compared to the rate of crystal growth (Butler and Rickard, 2000). Such conditions are produced when the solution is supersaturated with respect to the iron sulfide mineral (Butler and Rickard, 2000). In order to get supersaturated conditions, the ferrous iron and sulfide must be added to the system very quickly, such as occurs in the laboratory when the two solutions are mixed together. In a biowall, the production of sulfide and ferrous iron are controlled by the activity of sulfate-reducing bacteria, and iron-reducing bacteria (or possibly abiotic iron reduction), respectively. In order to create ferrous iron and sulfide quickly, the conditions for the bacteria must be favorable, providing sufficient useable organic carbon, sulfate, and favorable E_h -pH conditions. In addition, the conditions must remain at saturation with respect to iron sulfides to minimize or prevent Ostwald Ripening which can lead to formation of low surface area and relatively unreactive iron sulfides. Infiltration of surface water into biowall and resultant dilution is one such condition that should be minimized or eliminated.

Table ES-4 provides calculated percent chlorinated ethene removal and calculated first order rate constants for total chlorinated ethene removal for the different treatment systems. The data show that only the Altus AFB biowalls and the USEPA column constructed using biowall material from Altus AFB demonstrated significant chlorinated ethene removal. **Figures ES-7** and **ES-8** indicate the removal of chlorinated ethenes with abiotic and biotic signatures, respectively. **Figure ES-7** illustrates an abiotic signature at Altus AFB because accumulation of dechlorination products was not observed. **Figure ES-8** illustrates a biotic signature at Seneca Army Depot Activity because accumulation of dechlorination products was observed. While sampling and analysis of some of the sites at the time of this study did not provide evidence of biogeochemical transformation with an abiotic signature, significant chlorinated ethene removal with an abiotic signature was observed in the past. Thus the data from this single sampling event should not be used to make conclusions regarding the overall effectiveness of the biowalls implemented at the various sites.

ES-4 - Biogeochemical VOC Transformation and Controlling Parameters

Site	Well Pair (UG-Biowall)	Up-Gradient Total VOCs ($\mu\text{mol/L}$)	Down-Gradient Total VOCs ($\mu\text{mol/L}$)	% VOC Removal	First Order VOC Removal Rate Constant (h^{-1})	Median AVS (mg-S/kg)	Median CrRS (mg-S/kg) ^a	Volumetric Sulfate Loading ($\text{mg L}^{-1} \text{d}^{-1}$)	TOC (mg/kg)
Altus AFB OU-1	EPA-UMP1 - MP1	5.3	0.91	82.7%	6.3×10^{-3}	174	23	167	9.10%
Altus AFB SS-17 West Transect	B04U-BB04W	31	0.046	99.9%	1.1×10^{-2}	226	285	65	2.80%
Altus AFB SS-17 East Transect	B05U-BB05W	4.2	0.090	97.8%	6.3×10^{-3}				
USEPA Column	Influent-Effluent	20	0.30	98.5%	1.0×10^{-2}	1,450	1,518	98	4.20%
Dover AFB North Transect - DG Biowall	TS-MW02-TS- MW03	0.17	0.22	-36.7%	0 ^b	441	218	0.082	4.60%
Dover AFB South Transect - DG Biowall	TS-MW07 - TS- MW08	2.3	2.4	-6.9%	0 ^b	1,414	1,453	1.7 ^c	4.60%
Dover AFB North Transect - UG Biowall	TS-MW11 - TS- MW01	0.12	0.38	-204%	0 ^b	441	218	0.082	4.30%
Dover AFB South Transect - UG Biowall	TS-MW12 - TS- MW06	0.030	0.055	-91.5%	0 ^b	1,414	1,453	1.7 ^c	4.30%
Seneca Army Depot Activity Wall A	MWT-25 - TEMP- 1	0.38	0.96	-153%	0 ^b	64	181	4.6	6.0%
Seneca Army Depot Activity Wall B1	MWT-26 - MWT- 27	0.058	0.038	35%	4.3×10^{-4}	21	186	24	7.90%
Seneca Army Depot Activity Wall B2	MWT-27 - MWT- 28	0.039	<0.0005	>98.68%	4.4×10^{-3}			0.24	
Dugway Proving Ground	TW-25 - TW-28	10.6	11.4	-7.14%	0 ^b	80	43	NA	0.08%

Notes:

a) Reported CrRS values do not include AVS fraction.

b) Effluent concentrations were greater than influent concentrations so the rate constant was set to zero.

c) Does not account for sulfate loading from gypsum dissolution.

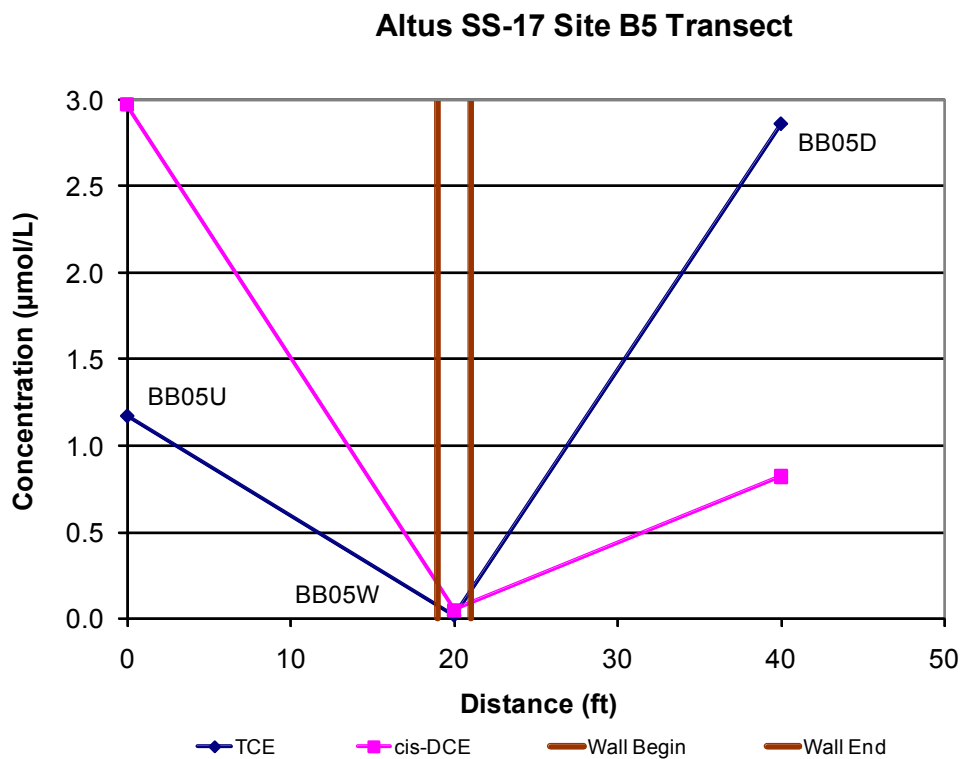
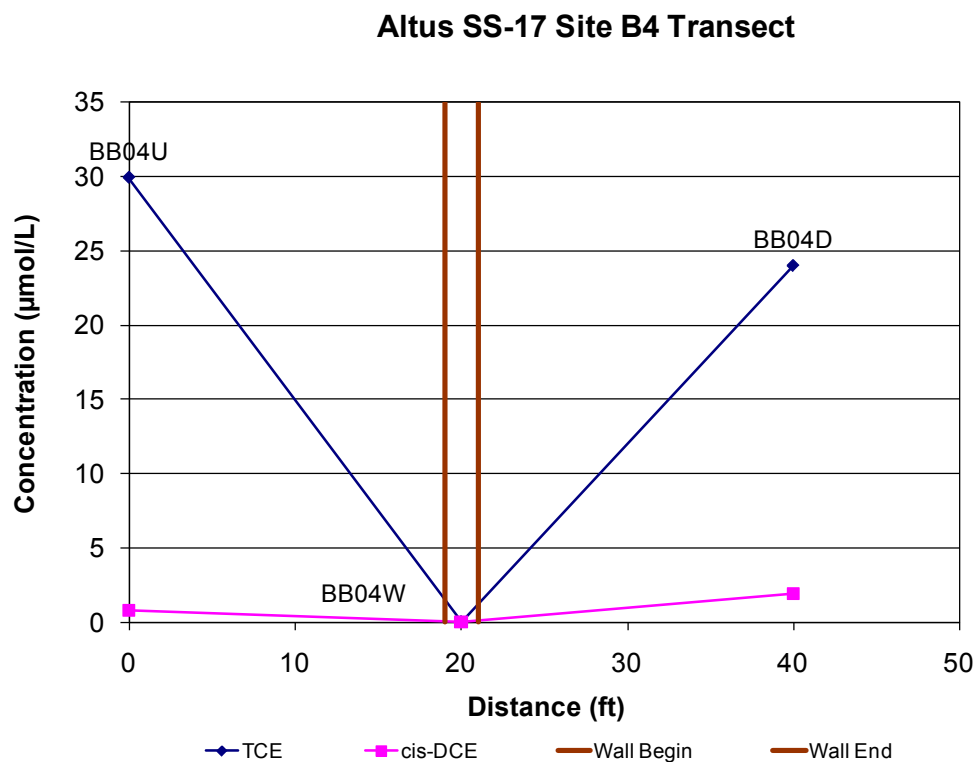


Figure ES-7 – Altus AFB SS-17 VOC Transects

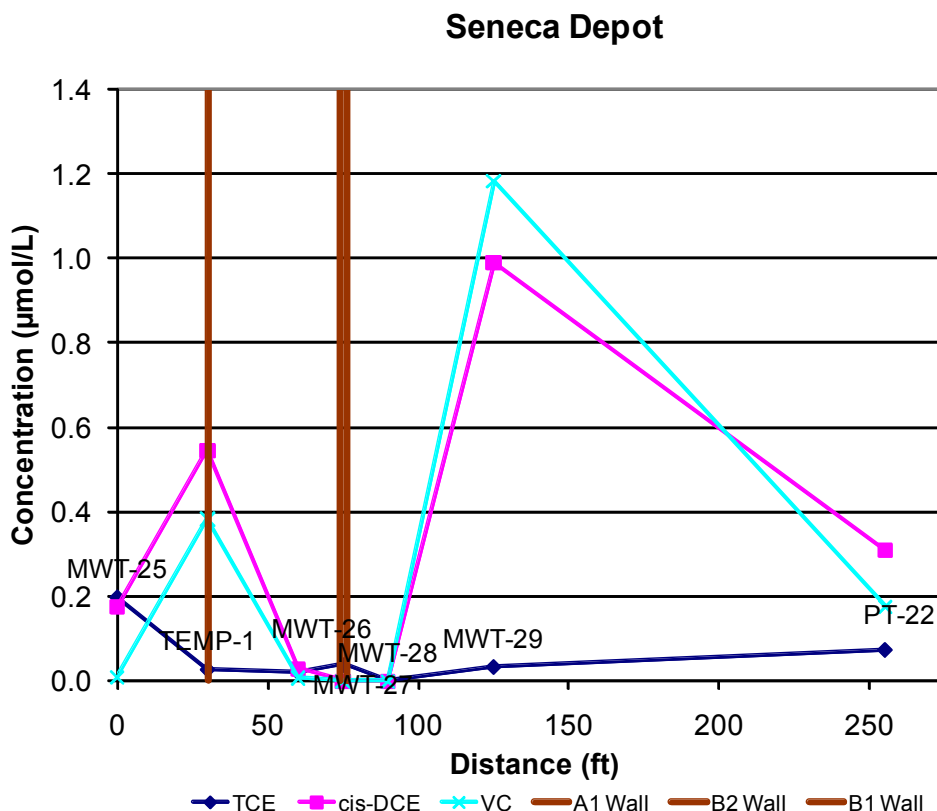


Figure ES-8 - Seneca Army Depot Activity VOC Transects

E3.2 Volumetric Sulfate Loading Rate

Comparison of the chlorinated ethene removal percentages and removal rates to the estimated iron sulfide concentrations based on bulk chemical extractions revealed no correlation as shown in **Table ES-4**. These data indicate that the presence of iron sulfides alone is insufficient to promote biogeochemical transformation. Volumetric sulfate loading rates were defined as the mass rate of sulfate to the biowall per unit volume of biowall and reported in units of milligrams per liter per day ($\text{mg L}^{-1} \text{d}^{-1}$) and values are presented in **Table ES-4**. The contribution of added gypsum was not included in this simple calculation because of complexity, but was likely an additional source of sulfate. Nevertheless, these data show that high sulfate volumetric loading rates were observed at the Altus AFB biowalls and the associated USEPA column but not at the other sites. Thus even though the Dover AFB biowalls had high iron sulfide concentrations, the volumetric sulfate loading rate was low and thus the potential for rapid generation of fresh iron sulfides was low. Gypsum was added to the southern portion of the Dover AFB biowalls which increased aqueous sulfate concentrations. However, the groundwater velocity at this site is very low and sometimes reverses direction; thus the potential for mixing is low which may have prevented reactive iron sulfide production. Furthermore, partial oxidation of iron sulfides as shown in **Figure ES-6** supports the conclusion that iron sulfides present in the Dover AFB biowalls were not freshly generated. Thus high chlorinated ethene biogeochemical transformation rate is dependent on both the presence of iron sulfides and a high volumetric sulfate loading rate to the biowall. A low volumetric sulfate loading rate leads to low sulfide production rates and can result in the rate of active iron sulfide formation being outweighed by

the rate of active iron sulfide aging to less reactive forms such as greigite. The following generic equation illustrates these concepts where high biogeochemical transformation rates of chlorinated ethene require that the rate constant k_1 be greater than k_2 :



The sulfide production rate is important because the production rate of active iron sulfides (i.e., k_1) must be sufficiently high to overcome their depletion rate (i.e., k_2), thus promoting accumulation of high active iron sulfide concentrations that can sustain biogeochemical chlorinated ethene dechlorination. Otherwise, the rate of production of active iron sulfides becomes the rate-limiting step and the active iron sulfides convert to inactive iron sulfide phases such as large diameter/low surface area particles or minerals such as greigite. In cases where sulfate is supplied by gypsum or other solid materials, (e.g., Altus AFB and Dugway Proving Ground sites), the volumetric sulfate loading rate may not be limiting provided sulfate dissolution and reduction is not rate limiting.

E3.3 Organic Carbon Content

Organic carbon is required to promote biological sulfate reduction and other bacterial processes. **Table ES-4** summarizes organic carbon contents for the solid media samples. Clearly 0.08 percent organic carbon was not enough, as illustrated by the Dugway site, but 2.8 percent was sufficient, as illustrated by the Altus AFB SS-17 site. The SS-17 mulch also had a low lignin content (4.7% for the tree mulch) making the organic carbon easier for the bacteria to break down into rapidly biodegradable monomers. In addition to solid sources of organic carbon, other sources including vegetable oil and soluble electron donors are also potentially applicable. Ultimately dissolved organic carbon must be made available to the bacteria responsible for the biogeochemical reactions. Sufficient organic carbon in combination with a high volumetric sulfate loading rate and a source of biologically or chemically reducible ferric iron appear to be critical factors that promote the ongoing production of high surface area iron sulfide minerals that drive *in situ* biogeochemical transformation processes.

E3.4 Strategies for Maximizing and Monitoring Biowall Performance

Table ES-5 summarizes critical factors that promote generation of high surface area iron sulfides that have sufficient reactivity with chlorinated ethenes. The factors which were identified in this study as important for *in situ* biogeochemical transformation of chlorinated ethenes include reduced iron phase mineralogy, iron oxide mineralogy, volumetric sulfate loading rate and organic carbon content. These factors should be considered when designing *in situ* biogeochemical transformation systems for remediation of chlorinated ethenes.

Table ES-6 summarizes several analytical techniques that are recommended for use in evaluating *in situ* biogeochemical transformation. These analytical techniques include methods for assessing the critical factors identified in **Table ES-5**. Additional parameters can also be useful and are discussed in the full report.

Table ES-5 – Summary of the Most Important Parameters Promoting Biogeochemical Transformation

Parameter	Optimal
Reduced iron phase mineralogy	Iron sulfides of mixed stoichiometry with high surface area. Forms can include iron sulfide particles, framboids, and/or iron sulfide coatings on iron oxides including magnetite.
Iron oxide mineralogy	Sufficient iron oxides are required to promote formation of iron sulfides. These iron oxides serve two purposes. One is to provide ferric iron that can be biologically or chemically reduced to ferrous iron that can complex with sulfide to form iron sulfides. Two is to provide a surface to which iron sulfides can attach.
Volumetric Sulfate Loading Rate	High to ensure constant renewal of reactive iron sulfides. Is accomplished through a combination of sulfate concentration and hydraulics necessary to generate a dynamic system.
Organic Carbon Content	Sufficiently high to promote anaerobic conditions and active sulfate reduction.

Table ES-6 – Analytical Techniques for Evaluating *In Situ* Biogeochemical Transformation

Analytical Technique	Data Generated	Data Use
Chemical extractions (AVS and CrRS)	Concentrations of bulk iron sulfides that vary in terms of elemental composition and surface area.	Determination whether iron sulfides are present in sufficient concentrations.
Electron microprobe (EMP)	Electron photomicrographs and elemental compositions.	Determination of mineral phases that are present and semi-quantitative indication of surface area.
Sulfate analysis (multiple methods available)	Calculation of volumetric sulfate loading in combination with the residence time.	Determination of whether sulfate loading is sufficiently high to promote rapid and on-going formation of fresh iron sulfide phases.
Tracer study (estimation of residence time)	Calculation of volumetric sulfate loading in combination with sulfate concentrations.	Determination of whether sulfate loading is sufficiently high to promote rapid and on-going formation of fresh iron sulfide phases.
Total and dissolved organic carbon	Organic carbon dissolved in groundwater that can be used as an electron donor and total organic carbon in the solid matrix that provides a long-term supply of dissolved organic carbon..	Determination of whether sufficient organic carbon is present to promote biogeochemical reactions.
Dissolved gases	Dissolved ethene concentration in groundwater.	Determine whether chlorinated ethene degradation is via reductive dechlorination. Must be used with caution since ethene is easily volatilized.
Dissolved chlorinated ethenes	Concentrations of PCE, TCE, cis-DCE, and VC in groundwater.	Determine presence of an abiotic signature.

E3.5 Conceptual Model of *In Situ* Biogeochemical Transformation

Figure ES-9 presents a hypothetical conceptual model of *in situ* biogeochemical transformation processes that may be occurring in the biowalls at Altus AFB. This model uses concepts presented previously (AFCEE et al., 2008) and observations made during the present investigation. The conceptual model includes multiple processes as described below:

- Biological sulfate reduction by sulfate-reducing bacteria that is driven by organic carbon resulting in formation of sulfide anions.
- Biological iron reduction by iron-reducing bacteria that is driven by organic carbon resulting in formation of ferrous cations and/or chemical reduction of iron indirectly driven by anaerobic biological processes the decrease the oxidation-reduction potential of the groundwater.
- Reaction of sulfide anions and ferrous cations to form ferrous sulfides.
- Precipitation and/or crystallization of ferrous sulfide to create iron sulfide particles potentially including framboids that have a high surface area and reactivity.
- Abiotic transformation of TCE or other chlorinated ethenes by iron sulfides to organic intermediates such as chloro-acetylene.
- Further abiotic transformation and/or biodegradation of the organic intermediates to carbon dioxide, water, and chloride anions.
- Generation of magnetite via abiotic processes or by biological iron reduction and subsequent reaction of ferrous cations with ferric iron oxides.
- Reaction of sulfide anions with naturally present magnetite or generated magnetite to result in formation of iron sulfide coated magnetite particles.
- Abiotic transformation of TCE or other chlorinated ethenes by iron sulfide coated magnetite to unidentified intermediates.

While this conceptual model requires further validation, the general concepts are considered to be an excellent starting point for: 1) establishing research needs to further the understanding of these processes, and 2) implementing and/or optimizing these processes in the field to facilitate cleanup of contaminated sites.

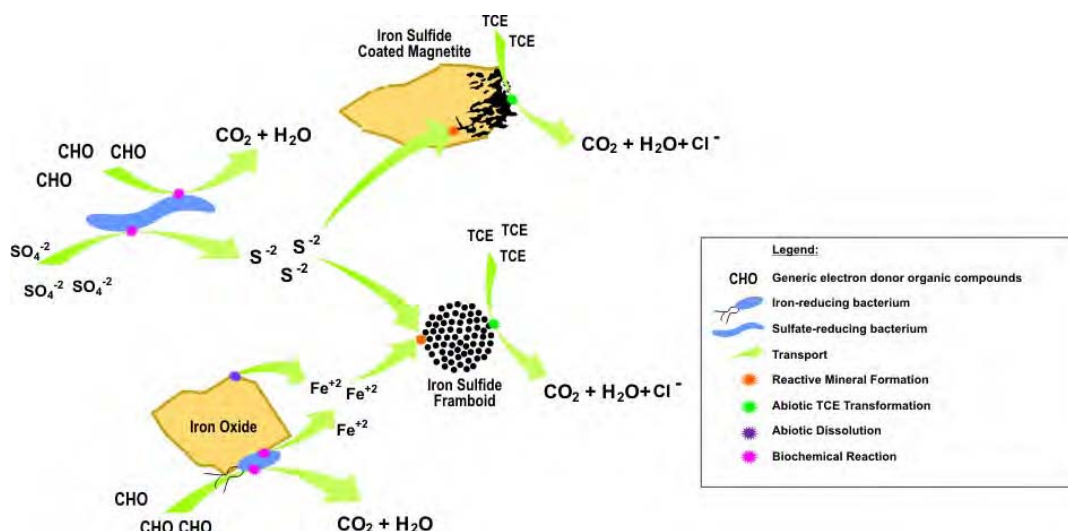


Figure ES-9 - Conceptual Biogeochemical Transformation Model

E4 Conclusions

The primary conclusions from this evaluation are as follows:

- The iron phases that were detected using the electron microprobe included iron minerals such as magnetite and hematite and various iron sulfides. The data also indicated that several iron sulfides were partially oxidized. The relative concentrations of total iron sulfides estimated by chemical extraction were generally consistent with the electron microprobe analysis results based on an estimated electron microprobe detection limit of about 200 mg/kg. These data indicate that the electron microprobe was a useful tool for identifying specific iron oxides and iron sulfides.
- The specific reactivity of framboidal pyrite may in fact have similar reactivity than iron monosulfide for a constant surface area. Thus the universe of iron sulfides responsible for *in situ* biogeochemical transformation of chlorinated ethenes appears to be broader than iron monosulfide.
- Geochemical modeling indicated that in general, iron oxides (e.g., magnetite and hematite) were undersaturated and thus could be expected to dissolve, and that iron sulfides (e.g., mackinawite, marcasite, troilite, greigite, and pyrite) were generally saturated or supersaturated and thus could be anticipated to form solid precipitates. Geochemical modeling provided an increased understanding of the potential to form specific reactive minerals and how these minerals would form at a given site. This understanding is important with respect to being able to design *in situ* biogeochemical transformation treatment systems because the specific mineral type and form directly control the rate of contaminant destruction. These data indicate that the presence of iron sulfides alone is insufficient to promote biogeochemical transformation.

- pH is very important with respect to controlling surface sites for the formation of iron sulfides and with respect to iron sulfide reactivity. Iron oxide minerals such as magnetite (at pH < 8.5) and hematite (at pH < 6.7) can provide surface sites for the formation of iron sulfides. Also, an increase in the pH from 6 to 8 can increase the rate constant by a factor of 5. The addition of specific iron oxides to the mulch can have a beneficial effect on biogeochemical transformation but must take aquifer pH into consideration.
- High chlorinated ethene biogeochemical transformation rate is dependent on both the presence of iron sulfides and a high volumetric sulfate loading rate to the biowall. A low volumetric sulfate loading rate leads to low sulfide production rates and can result in the rate of active iron sulfide formation being outweighed by the rate of active iron sulfide aging to less reactive forms such as greigite. Sufficient organic carbon in combination with a high volumetric sulfate loading rate and a source of biologically or chemically reducible ferric iron appear to be critical factors that promote the ongoing production of high surface area iron sulfide minerals that drive *in situ* biogeochemical transformation processes. The presence of iron sulfides alone is insufficient to promote biogeochemical transformation.
- Another important factor in maximizing the rate of reaction between chlorinated ethenes and iron sulfides is the surface area of the iron sulfides. A decrease in the median grain size of the iron sulfide particles from 1 μm to 10 nm can increase the rate constant by 100 times. Although nanoparticles were not likely present in any of the field systems investigated in this study, several investigators have reported the production of nanoparticulate iron monosulfides by sulfate-reducing bacteria (Ohfuji and Rickard, 2006). Ostwald ripening can result in the loss of mineral surface area and reactivity and can be caused by infiltration of surface water into a biowall. Surface water infiltration can also lead to iron sulfide oxidation and loss of reactivity. Maintaining a dynamic system with a high volumetric sulfate flux is critical.
- The factors which were identified in this study as important for *in situ* biogeochemical transformation of chlorinated ethenes include reduced iron phase mineralogy, iron oxide mineralogy, volumetric sulfate loading rate and organic carbon content. These factors should be considered when designing *in situ* biogeochemical transformation systems for remediation of chlorinated ethenes.

1.0 Introduction

Biogeochemical transformation is defined as “processes where contaminants are degraded by abiotic reactions with naturally occurring and biogenically-formed minerals in the subsurface” (AFCEE et al., 2008). Biogenically-formed minerals are created in response to reactions such as iron and sulfate reduction and are particularly important, as these minerals are continuously replenished. As long as the rate of mineral production is at least as fast as the rate of consumption of the mineral via reaction with the contaminant(s) and/or transformation to less-reactive minerals, the system is self-perpetuating. Biologically-formed minerals capable of abiotic transformation reactions with contaminants occur in natural systems, such as organic-rich marine sediments (bay muds, estuaries, etc.) and swamps (Vallentyne, 1963). *In situ* biogeochemical treatment systems were envisioned as a means of exploiting such natural processes via engineered reaction zones in the subsurface, such as organic carbon-based permeable reactive barriers (i.e., biowalls) and injection of organic carbon (e.g., vegetable oil emulsions) into a contaminated aquifer.

The use of organic carbon-based permeable reactive barriers for treating chlorinated ethenes is an emerging technology that has shown its potential to be a more cost-efficient method of treatment versus more mainstream technologies (e.g., zero-valent iron media) (AFCEE, 2008). A carbon-based substrate such as plant mulch or vegetable oil is used to promote *in situ* biogeochemical transformation of chlorinated solvents such as trichloroethene (TCE) and tetrachloroethene (PCE) into benign end products such as carbon dioxide and water. Some of the minerals which have been found to degrade chlorinated solvents such as TCE include the iron monosulfide minerals mackinawite (Butler and Hayes, 1999 and 2001; Jeong and Hayes, 2007) and troilite (Sivavec et al., 1995), the iron disulfide pyrite (Weerasooriya and Dharmasena, 2001; Lee and Batchelor, 2002a), magnetite (Lee and Batchelor, 2002a; Ferrey, 2004), green rust phases (Lee and Batchelor 2002b, Christianson and Stipp, 2003; Maithreepala and Doong, 2005), and iron phyllosilicates such as biotite (Lee and Batchelor, 2004).

As *in situ* biogeochemical treatment systems are still under development and few field-scale systems have been completed, many questions remain to be answered before the technology can gain regulatory acceptance and widespread use.

In April 2007 the Environmental Security Technology Certification Program (ESTCP) funded a workshop that was facilitated by the Naval Facilities Engineering Service Center (NFESC), the Air Force Center for Engineering and the Environment (AFCEE) and the United States Environmental Protection Agency (USEPA) in which 30 experts from around the country participated (AFCEE et al., 2008). The workshop was convened to discuss the current understanding of *in situ* biogeochemical transformation processes and identify research and demonstration needs. This investigation is an effort to meet some of the data needs and recommendations suggested by the workshop participants.

1.1 Objectives of Study

1.1.1 Objectives for Technology Development

The objectives for the development of the technology into a practical remedy that is recognized by regulatory agencies include the following:

- Develop design specifications for engineered systems utilizing *in situ* biogeochemical transformation.
- Determine how to optimize the systems under different geochemical and hydrogeological conditions.
- Recognize applications where satisfactory system performance will require an active operations and maintenance component (i.e., substrate and/or sulfate injection).
- Determine system life in terms of maintaining hydraulic conductivity and effectiveness with the aim of developing long term operations and maintenance cost estimates.

1.1.2 Objectives for the Investigation

Following up on the findings and recommendations of the workshop in 2007 (AFCEE et al., 2008), the Environmental Security Technology Certification Program (ESTCP), the NAVFAC Engineering Service Center (NFESC), the Air Force Center for Engineering and the Environment (AFCEE) and the United States Environmental Protection Agency (USEPA) evaluated five existing treatment systems where biogeochemical transformation processes may be occurring. The evaluations used a combination of conventional (i.e., methods commonly used in environmental investigations) and unconventional analyses and techniques (i.e., analyses used mainly for research). The sampling plan for the joint study has been published separately (Parsons, 2008).

The objectives of this study included:

- Evaluate methods to investigate the iron and sulfide mineralogy of the *in situ* biogeochemical treatment systems and subsurface soil materials.
- Perform and evaluate the utility of these methods to improve the understanding of biogeochemical reduction, including differentiation from biotic reductive dechlorination.
- Determine the conditions under which the potential for formation of appropriate forms of iron sulfides and biogeochemical reduction of chlorinated solvents to occur is optimal.
- Investigate and recommend a set of analyses to evaluate degradation of chlorinated solvents by biogeochemical transformation.
- Use the information gained from this investigation to develop practical guidelines for designing and optimizing substrate amendments (e.g., iron or sulfate) to stimulate biogeochemical reduction for differing geochemical and hydrogeologic conditions.

1.2 Approach

The approach to this effort followed the three basic lines of investigation proposed by Brown et al. (2007), which are as follows:

- Abiotic footprints.
- Plume degradation patterns.
- Mineralogical characterization.

In addition innovative approaches, such as the use of the electron microprobe and carbon stable isotope analysis were also evaluated.

The abiotic degradation pathway leads to a different set of end products through a different set of intermediate compounds than for biotic transformations. As a result, the footprint of abiotic degradation is distinct from the footprint of biological transformation (Brown et al., 2007). For example, anaerobic biological reductive dechlorination of TCE includes stepwise and successive dechlorination reactions to *cis*-1,2-dichloroethene (*cis*-1,2-DCE), vinyl chloride (VC), and ethene. Abiotic dechlorination typically does not follow the same stepwise dechlorination and the intermediates *cis*-1,2-DCE and VC are not observed. The distinctive footprint for abiotic degradation can be recognized by determining the trend in the concentrations of various transformation end products along the axis of the plume. The chlorinated solvents in water at the downgradient end of a plume have been subject to degradation for a longer period of time than the solvents in water very near the source. If the reaction products degrade more slowly than the parent contaminant then the relative concentrations of the reaction products will increase with distance. A buildup of daughter products is characteristic of biological transformation of PCE and TCE, and provides a footprint for biological degradation. When the reaction products are also rapidly transformed, the concentrations of all compounds decrease with distance (i.e., there is no buildup of daughter products). Such a plume pattern is characteristic of abiotic transformation.

The mineralogy of the treatment systems was characterized to identify the properties of the reactive mineral phases in the most effective systems. The chemical identify of the reduced iron minerals that were physically associated with the substrate (the source of organic carbon) were identified and characterized with respect to their degree of crystallinity, quantity, grain size, and morphology, all of which may contribute to system performance. The mineralogical characterization was conducted using unconventional analytical techniques, such as the electron microprobe.

In addition to the basic lines of investigation described above, the inorganic geochemical processes that are occurring within the systems were investigated using chemical equilibrium computer modeling. The modeling helped to understand the inorganic chemical reactions occurring within the treatment zones and the upgradient and downgradient groundwater.

An analysis of the stable carbon isotopes was also performed in order try to determine the degradation pathway (i.e., biotic versus abiotic) taking place at each site.

1.3 Background

Sites were selected for this investigation based on the following criteria (Parsons, 2007c):

- Sites with sustained anaerobic conditions suitable for the formation of reduced iron sulfides. In particular, mulch biowalls or emulsified vegetable oil applications.
- Sites with high sulfate concentrations, either natural or stimulated by addition of sulfate.
- Sites with evidence of bioavailable iron, such as soluble ferrous iron in ground water, or the intentional addition of material to the reactive matrix that had high content of bioavailable iron.
- Sites exhibiting substantial reductions in PCE, TCE, or cis-1,2-DCE without accumulation of cis-1,2-DCE, VC, or ethene; or sites where conditions are suitable for the production of reduced iron sulfides but where no evidence of substantial degradation of PCE or TCE exists.

Based on these criteria, the following sites were selected:

- The Operable Unit 1 (OU-1) and Spill Site 17 (SS-17) mulch biowalls at Altus Air Force Base (AFB), Oklahoma.
- The WP-14 mulch biowall at Dover AFB, Delaware.
- The Ash Landfill mulch biowalls at Seneca Army Depot Activity, New York.
- An emulsified vegetable oil pilot test at the Solid Waste Management Unit 97 (SWMU-97) Site, Dugway Proving Ground, Utah.

A description of each site is presented in the following sections, while a summary of the treatment system design, geochemical conditions and other information for each site is provided in **Table 1-1**.

Table 1-1 - Summary of System Design Parameters and Background Information for Each Site

Location	Installation Date	Dimensions	Biowall Composition ^a	Residence Time (days)	Historic VOC Concentrations (µg/L) ^b	Background Geochemistry^c
Altus AFB (OU-1 site), Oklahoma	July 2002 (pilot)	455 feet long by 24 feet deep by 1.5 feet wide.	Tree mulch (48%), cotton gin compost (10%), river sand (42%).	9-13.7	TCE: 8,000 DCE: 1,800 VC: Non-detect prior to installation	DO: 0 to 2 mg/L ORP: 0 to +150 mV Sulfate: 1,500 to 2,000 mg/L
Altus AFB (SS-17 site), Oklahoma	March-May 2005 (full-scale)	5,400 feet wide by 35 feet deep by 2 feet wide.	Tree mulch (42%), cotton gin trash (11%), concrete sand (32%), 0.75 in. gravel (15%)	1-50	TCE: 31,800 DCE: 6,400 VC: 11,600	DO: 0 to 2 mg/L ORP: 0 to +150 mV Sulfate: 1,500 to 2,000 mg/L
Dover AFB (WP-14 site), Delaware North Transect	December 2004	Dual Wall 250 feet long by 25 feet deep by 2 feet wide.	Tree mulch (50%), silty river sand (45%), and limestone (5%).	130 (UG wall), 195-391 (DG wall)	PCE: 3,400 TCE: 930 DCE: 2,000 VC: 63 µg/L	DO: 1 to 5 mg/L ORP: +200 to +400 mV Sulfate: <25 mg/L
Dover AFB (WP-14 site), Delaware South Transect	December 2004	Dual Wall 250 feet long by 25 feet deep by 2 feet wide.	Tree mulch (50%), silty river sand (40%), limestone (5%), and gypsum (5%)	130 (UG wall), 195-391 (DG wall)	PCE: 3,400 TCE: 930 DCE: 2,000 VC: 63 µg/L	DO: 1 to 5 mg/L ORP: +200 to +400 mV Sulfate: <25 mg/L

Table 1-1 - Summary of System Design Parameters and Background Information for Each Site (cont.)

Location	Installation Date	Dimensions	Biowall Composition ^a	Residence Time (days)	Historic VOC Concentrations (µg/L) ^b	Background Geochemistry^c
Seneca Army Depot Activity (Ash Landfill site), New York	October 2006 (full-scale)	Single Double-Wide and Dual Biowall System. 1,500 linear feet, 10 to 15 feet deep by 3.0 to 6.0 feet wide.	Mulch (50%) and Sand (50%). Mulch (6,240 cubic yards) in upgradient biowall coated with 15,600 gallons of vegetable oil.	16-66	TCE: 2,000 DCE: 960 VC: 95	DO: 2 to 4 mg/L ORP: 0 to 100 mV Sulfate: 500 to 900 mg/L
Dugway Proving Ground (SWMU-97 site), Utah	November 2004 (pilot)	Four Injection Wells on 10-foot centers.	Direct Injection of Field Mixed Emulsion - approximately 3000 lbs. vegetable oil mixed with lecithin, sodium bromide, and site groundwater.	NA	TCE: 2,300 DCE: <1.0 VC: Non-Detect	DO: <1.5 mg/L ORP: <0 mV Sulfate: 10,470 mg/L

Notes:

a) By volume.

b) Contaminants are maximum concentrations prior to treatment or upgradient of treatment zone.

1.3.1 Altus AFB

OU-1 Site

The OU-1 biowall is 455-foot-long, 1.5-foot-wide, by 24-foot-deep, installed using a continuous trenching method. The biowall substrate consists of 48 percent tree mulch (deciduous and evergreen trees and shrubs), 10 percent cotton gin compost, and 42 percent river sand by volume. Ten groundwater and four soil vapor monitoring wells were installed by Parsons Infrastructure & Technology Group, Inc. (Parsons). Parsons conducted post-installation sampling of groundwater at the ten monitoring wells and existing monitoring wells OU-1-01 and WL019 in July 2002, September 2002, March 2003, November 2003, and April 2005. Additional monitoring wells were installed by the USEPA National Risk Management Research Laboratory/Ground Water and Ecosystems Restoration Division (NRMRL/GWERD) who collected additional monitoring data. A site map showing the biowall location, site features, and the monitoring network is provided in **Figure 1-1**. Additional information is provided in an AFCEE Technical Protocol (AFCEE, 2008).

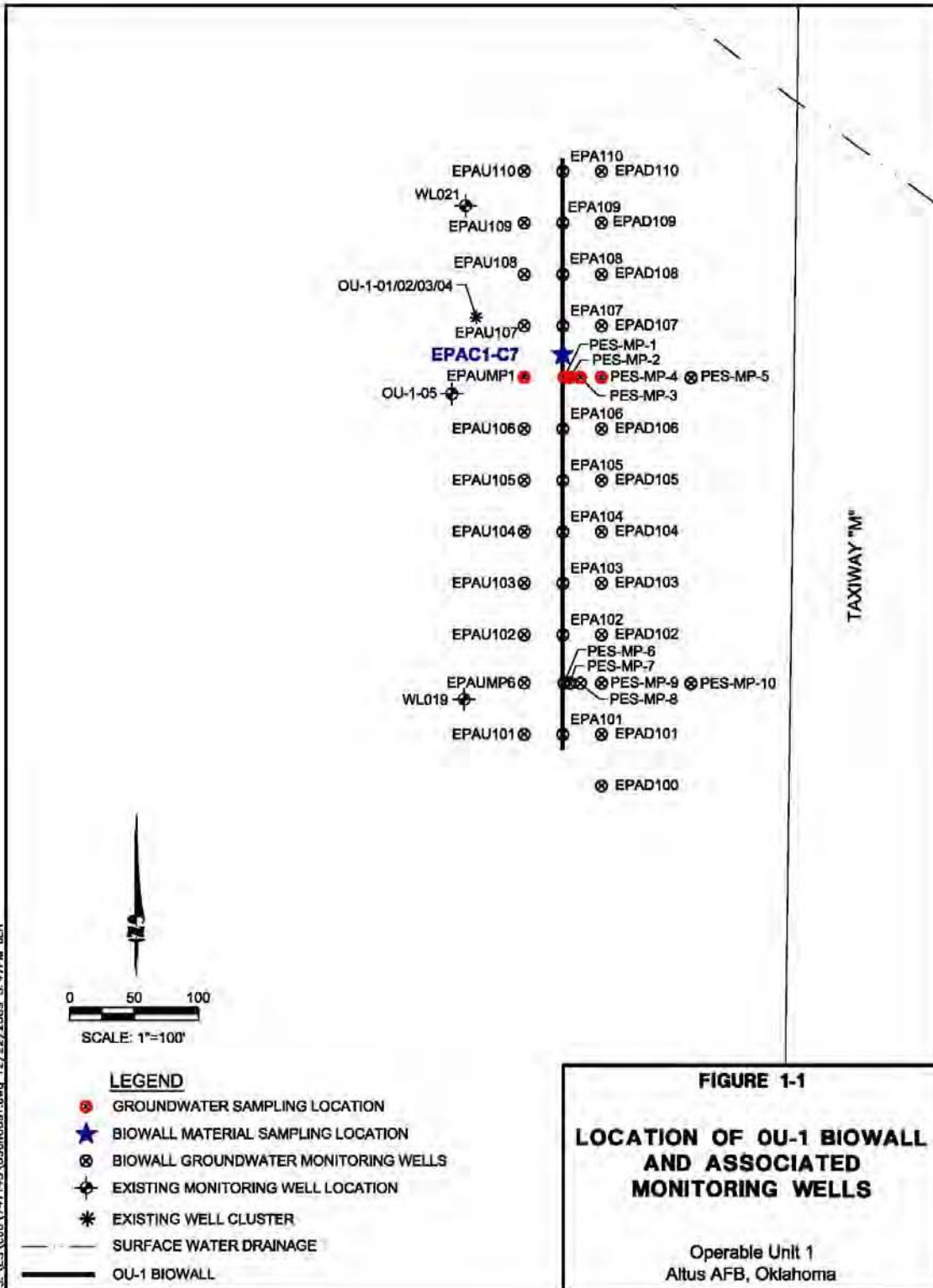
Hydrogeology

Depth to groundwater within the biowall ranges from 5.0 to 8.0 feet below ground surface (bgs), with the depth of the trench at approximately 24 bgs. Weathered and fractured silty clay extends to a depth of approximately 25 to 30 feet bgs, which is underlain by silt and dense shale of the Hennessey Group. The biowall does not extend to the top of the low permeability sediments of the Hennessey Group, and migration of groundwater underneath the biowall trench is likely to occur. In addition, the trench does not intercept the entire width of the chlorinated solvent groundwater plume. Mixing of groundwater passing through the biowall and contaminated groundwater running beneath or around the ends of the biowall may occur.

The rate of groundwater flow through the study area was estimated from an average hydraulic conductivity of the native soil of 8.7 feet per day (ft/day), an average hydraulic gradient across the demonstration site of 0.003 foot per foot (ft/ft), and an estimated value of 0.15 for the effective porosity of site soils (Parsons, 2007a). The average groundwater flow rate is approximately 0.17 ft/day or 63 feet per year (ft/yr).

The residence time of groundwater in the biowall can be estimated by dividing the width of the biowall (1.5 feet) by the average rate of groundwater flow of 0.17 ft/day, which results in a residence time of approximately 9 days. The USEPA NRMRL/GWERD performed a tracer test at the OU-1 biowall in 2005 to investigate residence time in the biowall, as well as hydraulic characteristics surrounding the wall. During this study the USEPA estimated seepage velocity in the aquifer as 0.2 ft/day (Lu et al., 2008). The measured effective porosity of the aquifer is 0.15, and the water filled porosity of the biowall is 29 percent (John Wilson, USEPA NRMRL/GWERD, personal communication). Under these conditions, the expected residence time in the biowall trench is approximately 10 days.

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An average decrease in the concentration of TCE of over 99 percent was observed within the biowall relative to upgradient monitoring locations over the first 24 months following installation, with little evidence of an accumulation of *cis*-1,2-DCE or VC. Between 24 months and 34 months post installation, the average concentration of TCE in the biowall decreased to approximately 96 percent relative to upgradient locations. However, as of April of 2005 four wells within or immediately downgradient of the biowall still had concentrations of TCE less than the USEPA maximum contaminant level (MCL) for drinking water of 5.0 micrograms per liter ($\mu\text{g/L}$).

Historic System Performance

In July 2004, the average reduction in the total molar concentration of chloroethenes within the biowall was 73 percent, decreasing to 31 percent during the April 2005 sampling event. This suggests that *cis*-1,2-DCE is also being degraded, but that the degradation of *cis*-1,2-DCE within the biowall may be less effective over time or is masked by potential transformation of TCE to *cis*-1,2-DCE upgradient of the biowall.

Concentrations of VC along a well transect in the northern portion of the biowall increased by approximately two orders of magnitude between 24 months and 34 months post installation. The presence of elevated concentrations of *cis*-1,2-DCE and VC may be due, in large part, to sequential anaerobic dechlorination of TCE occurring in an upgradient bioreactor (Parsons, 2006a). The decrease in percent reduction of total molar concentrations observed between July 2004 and April 2005 may indicate that the biowall is less effective in degrading *cis*-1,2-DCE and VC than it is at degrading TCE.

Geochemical Conditions

During the first 16 months of the demonstration background geochemical conditions were weakly aerobic with concentrations of dissolved oxygen ranging from less than 0.1 mg/L to 1.9 mg/L, and oxidation-reduction potential ranging from approximately +213 millivolts (mV) to +354 mV (referenced to the standard hydrogen electrode [SHE]).

Beginning around November 2003, the OU-1 biowall began to receive groundwater originating from the LF-03 bioreactor within Landfill 3 that was installed upgradient of the OU-1 biowall in October 2003. The result is that groundwater entering the northern portion of the biowall is more reducing and contains a higher percentage of the dechlorination products *cis*-1,2-DCE and VC. During the July 2004 and April 2005 sampling events, groundwater geochemistry upgradient of the northern portion of the biowall became moderately anaerobic with oxidation-reduction potential values in the range of -90 mV to -130 mV.

Background concentrations of native electron acceptors are considered high at this site, with sulfate present at 1,600 to 2,000 mg/L. While beneficial for the production of reduced iron sulfides, sulfate reduction may utilize available substrate (electron donor) at the expense of biotic reductive dechlorination of chlorinated ethenes.

Geochemical data collected from within and downgradient of the biowall during the course of the demonstration indicate that geochemical conditions were rapidly altered to a reducing environment conducive for anaerobic degradation of chlorinated ethenes. Concentrations of dissolved oxygen were reduced to below 1.0 mg/L within the biowall within 4 weeks of

installation, and to below 1.0 mg/L downgradient from the biowall within two months of installation. Oxidation-reduction potential measurements indicate that groundwater became sufficiently reducing to support iron-, manganese-, and sulfate-reduction. Methane concentrations were also elevated indicating methanogenesis had also been stimulated. Oxidation-reduction potential conditions remained strongly reducing through sampling in April 2005.

Monitoring results for the OU-1 permeable mulch biowall over a period of 34 months indicate that highly reducing conditions have been established and sustained within and downgradient of the biowall system (Parsons, 2007a). The primary terminal electron accepting processes appear to be sulfate reduction, with methanogenesis also evident.

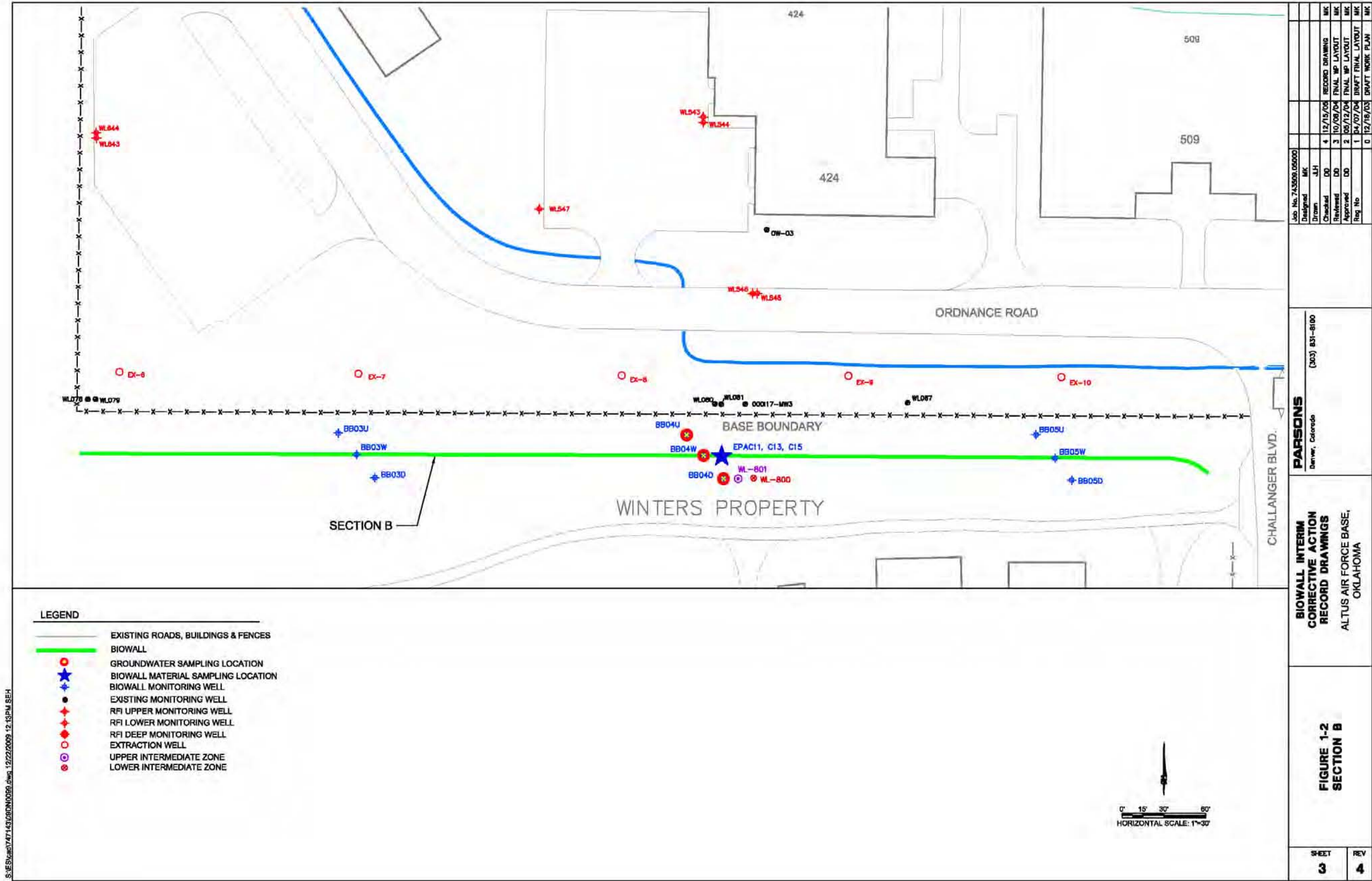
Concentrations of total organic carbon within the OU-1 biowall system have remained elevated, ranging from approximately 25 to 100 mg/L for locations within and up to 10 feet downgradient of the biowall. Data for chlorinated ethenes indicates that anaerobic degradation (reductive dechlorination and biogeochemical reduction) was occurring as of April 2005 (34 months post installation). Additional monitoring by the USEPA NRMRL/GWERD in March 2006 and April 2007 indicate the biowall continues to be effective in degrading TCE within the biowall.

Analysis of the mulch backfill material in 2003 by Earth Science Services, Inc. and Rowan University (Kennedy and Everett, 2003) and again by Parsons in April 2005 (Parsons, 2007a) indicates that significant amounts of iron and sulfide bearing minerals are present in the biowall backfill, which enables the precipitation of reduced iron sulfide minerals. Thus, biogeochemical reduction appears to be a viable degradation process within the biowall with reduced sulfides continuing to be present as of the April 2005 sampling event. Additional details can be found Appendix F.2 of the Biowall Protocol (AFCEE, 2008).

SS-17 Site

The biowall system at SS-17 was installed as an interim corrective action to limit off-site migration of chlorinated ethenes dissolved in groundwater by enhancing anaerobic degradation. Approximately 5,800 feet of overlapping biowall segments having a width of 24 inches were installed to a maximum depth of 35 feet bgs. The biowall was backfilled to within two feet of the surrounding ground surface with a mixture of mulch (42 percent), concrete sand (32 percent), 0.75-inch gravel (15 percent), and cotton gin trash (11 percent). The primary contaminants of concern (COCs) include TCE, *cis*-1,2-DCE, VC, and carbon tetrachloride.

Groundwater sampling was a coordinated effort between the US Air Force via Parsons and the USEPA NRMRL/GWERD. A baseline groundwater sampling event was performed in May 2004, and seven quarterly groundwater post-biowall-installation sampling events were performed from July 2005 to January 2007. In addition, samples of biowall backfill material and native soil were collected in October 2006 in cooperation with the USEPA NRMRL/GWERD. The objective of this activity was to analyze the chemistry and mineralogy of the native soils and biowall material for evaluation of the occurrence of biogeochemical reduction of chlorinated ethenes. A site map showing the biowall location, sampling locations, site features, and the monitoring network is provided in **Figure 1-2**.



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As part of the proposed study, biowall samples were collected using a modified sampling method for collecting frozen core material. Samples were collected by the USEPA NRMRL/GWERD from the B4 well transect of the B Section in September 2007. Section B is 832 feet long at the ground surface and 782 feet long at the base of the wall. Section B receives the highest concentrations of chlorinated ethenes of any of the Base boundary biowall segments because it cuts across the core of the SS-17 chlorinated ethene plume.

In addition, the mulch mixture in a 180-foot-long portion of Section B was supplemented with 48 tons of magnetite to increase the iron content of the sand from 1,600 mg/kg to 118,000 mg/kg to promote biogeochemical reduction of chlorinated ethenes. Well Transect BB04 was installed through this section and is used to evaluate the impact of the magnetite addition. The following subsections provide a brief description of site conditions at the B Transect.

Hydrogeology

Site stratigraphy for the SS-17 plume is similar to that described for the OU-1 biowall above. Using the geometric mean of site-wide hydraulic conductivities derived from slug tests across the SS-17 biowall site (7.0 ft/day), an average hydraulic gradient of 0.004, and an estimated effective porosity of 0.10, the calculated average advective groundwater seepage velocity in the surficial aquifer at SS-17 is 0.28 ft/day (102 ft/yr) (Parsons, 2007b). Using the range of hydraulic conductivities derived for the surficial aquifer (1.0 to 24 ft/day) yields groundwater seepage velocities of 0.04 ft/day (15 ft/yr) to 1 ft/day (365 ft/yr). Given a biowall thickness of two feet results in a residence time of 2 to 50 days (assuming the groundwater velocity through the wall is the same as for the aquifer).

Historic System Performance

Reductions in concentrations of TCE from upgradient to within the biowall ranged from 42.9 percent to 99.4 percent over time, with an average reduction of 94 percent. Since October 2005, the average percent reduction of TCE from upgradient to within the B biowall has been at least 84 percent, and the reductions calculated for each of the two most recent sampling events (October 2006 and January 2007) range from 94 percent to 99 percent. As of January 2007, there was no evidence of a decrease in the TCE removal efficiency of the B Section biowall.

On average, TCE concentrations decreased by only six percent from upgradient to downgradient of biowall Section B, indicating substantial rebound due to desorption and back-diffusion of TCE from the aquifer matrix downgradient of the B biowall. An unusually large increase in TCE concentration from upgradient to downgradient of the biowall occurred at Transect BB04 in October 2006 (5,668 µg/L to 8,365 µg/L). Excluding this increase, the TCE concentration from upgradient to downgradient at the B biowall decreased by an overall average of 43 percent.

Average concentrations of *cis*-1,2-DCE were relatively stable across the biowall, while concentrations of VC increased substantially from upgradient to within the biowall. An increase in VC indicates that *cis*-1,2-DCE being produced within the biowall is being rapidly dechlorinated to VC.

Geochemical Conditions

Oxidation-reduction potential within the B Section biowall has ranged from +85 mV to – 278 mV over time from July 2005 to January 2007. The primary terminal electron accepting

processes at the B Section biowall are sulfate reduction and methanogenesis. In January 2007, sulfate concentrations upgradient of the biowall ranged from 908 mg/L to 1,410 mg/L, and within the biowall ranged from 540 mg/L to 1,330 mg/L. Sulfate concentrations rapidly rebound downgradient of the biowall, likely due to the presence of gypsum or anhydrite in native sediments. Concentrations of methane within the biowall have ranged up to 18 mg/L.

Biogeochemical data indicates that highly reducing conditions were established and sustained in the B biowall section throughout the sampling period, despite the fact that concentrations of dissolved organic carbon in the biowall were decreasing over time. This observation is supported by the maintenance of highly negative oxidation-reduction potentials, the lack of increasing trends in sulfate concentrations (within the biowall), and a lack of decreasing trends in methane concentrations over time.

The TCE removal efficiency of the B biowall from October 2005 to January 2007 ranged from 84 percent to 99 percent and was typically at least 94 percent. TCE removal rates in the biowall do not appear to have been consistently increasing or decreasing over time after October 2005. Removal of the TCE was accompanied by enhanced microbial production of *cis*-1,2-DCE and VC.

The total molar concentration of chlorinated ethenes decreased by an average of 18 percent from upgradient to within the biowall from July 2005 to January 2007 indicating some transformation of chlorinated ethenes to non-toxic end products. However, significant rebound in total molar chlorinated ethene concentrations occurred downgradient of the biowall, most likely due to desorption and back-diffusion of chlorinated ethenes from the aquifer matrix downgradient of the biowall. As a result, there was an overall average increase of approximately 11 percent in total molar chlorinated ethene concentrations from upgradient to downgradient locations. However, if a relatively high-magnitude rebound in the total molar chlorinated ethene concentration that occurred at Transect BB04 in October 2006 is excluded, then the total molar concentration of chlorinated ethenes from upgradient to downgradient of the biowall decreased by an overall average of about 30 percent.

Ferrous iron and sulfide data suggest that these two metabolic byproducts of microbial utilization of the mulch backfill may be precipitating in the form of reactive iron sulfide minerals. However, the degree to which biogeochemical reduction is occurring at the B biowall is difficult to quantify.

Column Study

Shen and Wilson (2007) performed a column study using the same biowall mulch materials and proportions as used for the SS-17 site at Altus AFB, as well as additional columns supplemented with hematite and hematite plus limestone. The study was performed to determine the abiotic and biological transformation rates of chlorinated solvents and to better define the mechanisms and reactions taking place under controlled flow conditions. The columns used in the study were large; 15 centimeters (cm) in diameter (5.9 inches) by 46 cm in length (18.1 inches), which should have minimized edge effects (flow along the mulch-column interface as opposed to porous media flow through the material) which are more pronounced in narrower columns with a smaller cross-sectional area. The flow was set at 0.2 L/d, resulting in a residence time of about 17 days. TCE was spiked into site groundwater to obtain a constant influent concentration near

20 micromolar (μM , 2,585 $\mu\text{g/L}$ on 5/15/07). In order to determine the fate of TCE in the system, ^{13}C tagged TCE was used as the spike material for a period of time. The concentration of ^{13}C was determined in methane, and dissolved inorganic carbon in the column effluent. The overall reaction rate constant for each column (biotic and abiotic) was calculated from the residence time and influent and effluent TCE concentrations assuming a pseudo first-order rate equation. The fraction of the transformation attributable to abiotic degradation was calculated by assuming that the amount of iron sulfide retained in the columns was proportional to the abiotic transformation rate and that the biological transformation rate and degree of adsorption was the same in all of the columns. The authors also calculated an abiotic rate. A plot of the overall reaction rate constant versus the iron sulfide retained for each column would result in a positive correlation, and the point of intersection of the line or curve with the overall reaction rate axis would be the biotic part of the overall rate.

A few of the observations and conclusions of the study were as follows:

- Pseudo first order rate constants for TCE transformation ranged from 0.20 to 0.55 day^{-1} , which is about one to two orders of magnitude slower than for zero valent iron walls.
- Approximately 50 to 88 percent of the TCE transformation was due to abiotic processes and 12 to 50 percent to biological processes.
- Less than one percent of the TCE that was removed in the mulch columns could be accounted for as cis-1,2-DCE. Most of the TCE (53 percent) was removed as CO_2 .
- Concentrations of the possible daughter products acetylene, vinyl chloride, 1,1-DCE, trans-1,2-DCE, ethene, and ethane were either always below the method detection limit, were infrequently detected, or were very low and insignificant.
- Mass balance calculations showed that sulfur was being removed within the columns. Because a black precipitate was observed in the flow channels of the columns, the mechanism was proposed to be removal as iron sulfides (specifically FeS). This was confirmed by analyzing the contents of one of the columns (He et al., 2008).
- The sulfide concentrations in the effluent from the columns containing hematite were below the analytical detection limit, suggesting that in these columns the rate of precipitation of iron sulfide was controlled by the rate of sulfate reduction within the system.
- After 157 days of operation the rate of iron sulfide accumulation decreased for the columns without hematite, probably because all of the iron(III) in the matrix had all been reduced to iron(II).
- A pathway for abiotic transformation of TCE to carbon dioxide by FeS was proposed which takes place in three stages; first acetylene is produced by the abiotic reaction, then the acetylene is fermented to ethanol and acetate, which in turn are oxidized to carbon dioxide by sulfate-reducing bacteria.
- A second abiotic transformation pathway produces cis-1,2-DCE (as does biological transformation), which is also believed to react with FeS to produce acetylene, which is then in turn fermented to ethanol and acetate which are oxidized to carbon dioxide.

Several samples (7 slices) from Column B3 (biowall mulch with added hematite) were provided for this investigation (see He et al. 2008 for further characterization of acid volatile sulfide [AVS] and chromium reducible sulfide [CrRS] in the column).

1.3.2 Dover AFB (Site WP14)

The biowall demonstration at Site WP14 was initiated in December 2004 by installing approximately 550 linear feet of mulch biowall in two parallel biowall sections, each 1.5 feet wide, and installing 12 groundwater monitoring points. The mixture for the northern half of the biowall consisted of tree mulch (50 percent), silty river sand (45 percent), and limestone (5 percent), while the southern half mixture was composed of tree mulch (50 percent), silty river sand (40 percent), limestone (5 percent), and gypsum (5 percent). A site map showing the biowall location, site features, and the monitoring network is provided in **Figure 1-3**. AFCEE via Parsons, with the support of Dover AFB, the Dover AFB National Test Site, and URS Corporation, conducted nine groundwater monitoring events over a period of 12 months following biowall installation.

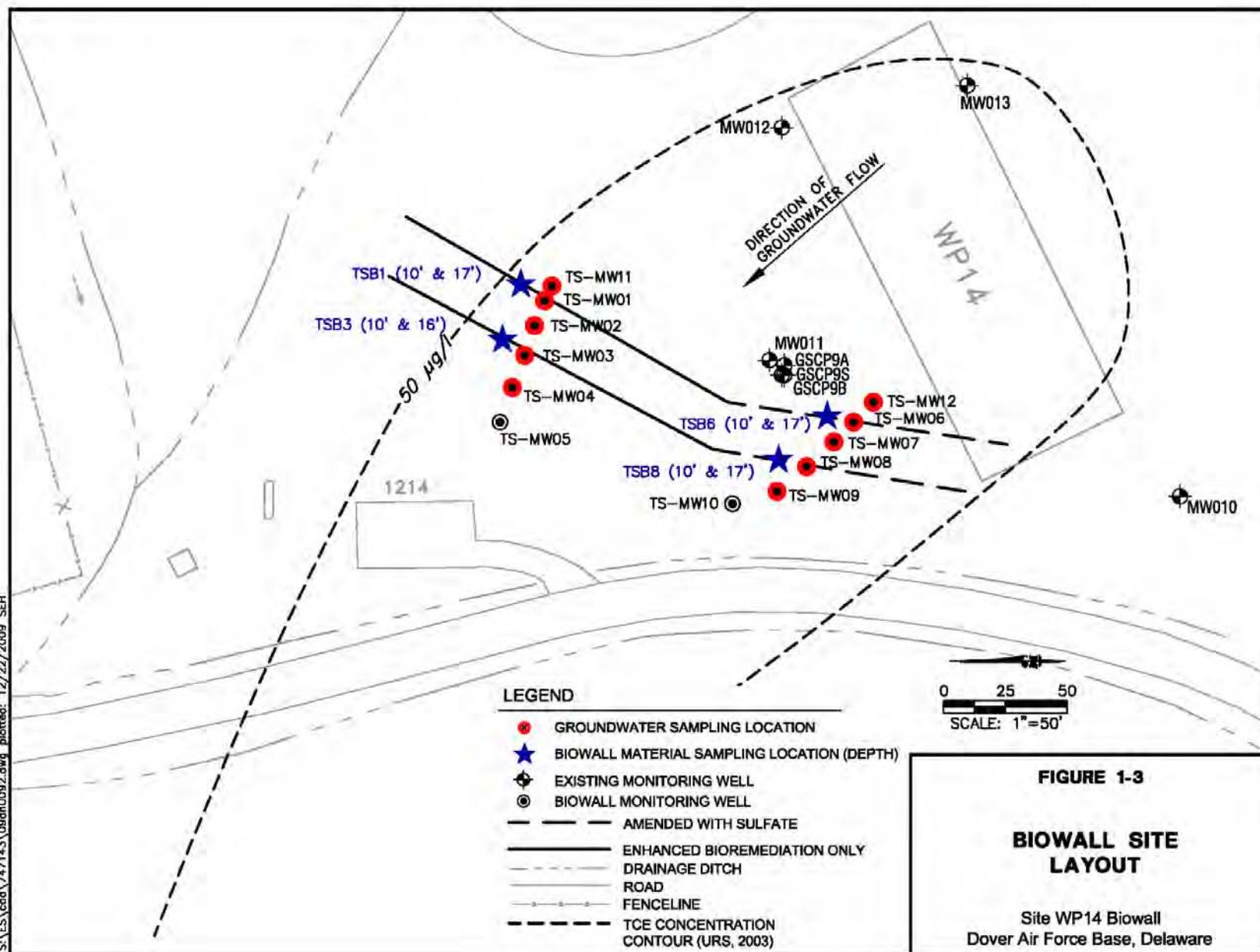
Hydrogeology

The depth to groundwater at the WP14 site typically ranges between approximately 5 and 9 feet bgs. The depth of the bottom of the biowall backfill is approximately 23 to 25 bgs. Therefore, the saturated thickness within the biowall ranges from 17 to 19 feet at any given time, depending on seasonal variations in groundwater levels.

The last round of groundwater elevation data was collected on October 3, 2005 for the biowall wells, as well as a selection of surrounding base monitoring wells. Inspection of well completion data for monitoring wells MW010, MW011, MW012, and MW013 shows the well screen intervals are very long, ranging from 45 to 50 feet, and that they fully penetrate the surficial aquifer to depths of 55 to 62 feet bgs. The biowall study wells are only screened from 18.5 to 23 feet bgs. The United States Geological Survey (USGS) determined that significant downward flow exists in the surficial aquifer beneath the WP-14 Site (USGS, 1998 and 2002). Therefore, groundwater elevation data collected from MW010, MW011, MW012, and MW013 are not suitable for comparison to data collected from the remainder of the wells in the study area. For example, the water table at location GSCP9A is typically 2.5 to 3.0 feet higher than at MW011, installed only 9 feet away.

Ignoring data collected from MW010, MW011, MW012, and MW013 (for the reasons stated above), the groundwater elevation data collected during October 2005 and December 2005 indicates that the groundwater potentiometric surface in the study area is very flat and slopes toward the northwest. Note that groundwater elevation highs have occasionally been observed at the monitoring wells installed within the biowalls (e.g., TS-MW03 and TS-MW06 in October 2005). These temporary highs within the biowalls are possibly a result of surface water recharge through the biowall backfill material.

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Short term reversals in groundwater flow or mounding of groundwater around the biowalls may be possible during periods of heavy precipitation due to surface water recharge. Thus, it is possible that monitoring wells installed upgradient of the biowalls (TS-MW11, TS-MW12, GSCP9A) have been impacted sporadically by the biowall system. It is unlikely that any reversal in groundwater flow or mounding of the groundwater potentiometric surface would persist given the high transmissivity of the site soils and biowall backfill materials.

Slug tests were conducted immediately after biowall installation (December 2004) to ensure that the hydraulic conductivity of the biowall backfill material was higher than that of the surrounding native soil. During the December 2004 sampling event, the average hydraulic conductivity in the biowalls (TS-MW-3 and TS-MW-08) was approximately 2.0×10^{-3} centimeters per second (cm/sec), or 5.7 ft/day, while the average hydraulic conductivity in natural soils (TS-MW-04 and TS-MW-09) was 9.8×10^{-4} cm/sec or 2.8 ft/day. This data indicates that the hydraulic conductivity measured in the biowall backfill material was approximately 2 to 3 times that measured in native soil, indicating that the biowalls should not impede groundwater flow.

The hydraulic conductivity measured in the biowalls up to the December 2005 sampling event remained relatively stable, at approximately twice that of native soil. The hydraulic conductivity calculated from slug tests conducted in the biowalls during the December 2005 event was approximately 5.7×10^{-4} cm/sec (1.66 ft/day), which is less than half of the values previously observed in the biowalls. This is also similar to the hydraulic conductivity measured in native soil (1.58 ft/day) during the same event. It is possible that the observed reduction in hydraulic conductivity in December 2005 is due to settling and compaction of the biowall backfill material.

The rate of groundwater flow through the study area can be estimated from an average hydraulic conductivity of 1.58 ft/day, an average hydraulic gradient across the demonstration site of 0.0015 ft/ft, and an estimated effective porosity for native soil of 0.25. The resultant average groundwater flow velocity is approximately 5.6 ft/yr (0.015 ft/d). This rate of groundwater flow is considerably lower than the rates of groundwater flow estimated in the past (USGS, 1998 and 2002), mostly due to the flat hydraulic gradient observed in the study area. Dividing the wall thickness (i.e., 1.5 ft) by the flow velocity results in a residence time of 130 days for the upgradient (UG) wall and 195-391 days for the downgradient (DG) wall.

System Performance

Chlorinated ethene concentrations at TS-MW12, located upgradient from the south transect, were variable over time. Concentrations of chlorinated ethenes at background well TS-MW11, located upgradient from the north well transect, were relatively consistent over time.

Some of the variability in concentrations of chlorinated ethenes observed at TS-MW12 may have been due to an influence from the nearby biowall. Concentrations of total organic carbon measured in samples from TS-MW12 indicate that this location was impacted by soluble organic carbon from the biowall during a sampling event in June 2005. Over time it is more likely that the variability in concentrations of chlorinated ethenes observed at TS-MW12 results from natural variations in groundwater flow and migration of chlorinated ethenes. The dechlorination products *cis*-1,2-DCE and VC were detected at elevated concentrations at the upgradient

monitoring wells during the demonstration, suggesting that some reductive dechlorination did occur upgradient of the biowall.

During the 12-month monitoring period following biowall installation, PCE and TCE were largely dechlorinated to *cis*-1,2-DCE within the biowalls. Low concentrations of VC were detected, indicating some dechlorination of *cis*-1,2-DCE to VC occurred. Overall concentration trends indicate that the biowall system was unable to promote significant biotic dechlorination of *cis*-1,2-DCE to VC and ethene during the 12 month monitoring period. However, concentration data collected from the southern well transect indicates that significant reductions in PCE and TCE occurred without an accumulation of *cis*-1,2-DCE and VC, likely due to biogeochemical reduction. Sulfate in the form of powdered gypsum was added to the southern biowall segments to stimulate formation of reduced iron sulfide minerals.

Geochemical Conditions

Background geochemical conditions at the study site are moderately to strongly aerobic with concentrations of dissolved oxygen greater than 2 mg/L and with oxidation-reduction potential ranging from +371 mV to +449 mV. These geochemical conditions are not conducive to anaerobic degradation processes. Background concentrations of sulfate are less than 20 mg/L. Therefore, a source of sulfate was needed to stimulate sulfate reduction to induce the production of reduced metal sulfides.

Geochemical data collected from within the biowalls indicates that anaerobic conditions (i.e., dissolved oxygen less than 1.0 mg/L and oxidation-reduction potential less than 0 mV) were induced within approximately 1 to 2 weeks following biowall installation. During the December 2004 event, concentrations of dissolved oxygen within the biowalls averaged approximately 0.8 mg/L while oxidation-reduction potential averaged -34 mV. By approximately 4 weeks following biowall installation (January 2005), the oxidation-reduction potential became sufficiently reducing to support nitrate, manganese, iron, and sulfate reduction. Oxidation-reduction potentials remained in the range of -100 mV to -175 mV throughout the 12 month monitoring period.

Oxidation-reduction potentials measured at monitoring wells installed downgradient of the biowalls remained at or near background conditions during the monitoring period, indicating that the monitoring wells installed downgradient of the biowalls were only weakly impacted by geochemical effects induced by the biowalls. The predominant direction of groundwater flow in the study area was to the northwest, as expected, but at a very low rate of flow due to a flat hydraulic gradient. Upgradient monitoring wells TS-MW11 and TS-MW12 were apparently impacted by geochemical changes from the biowall during at least one sampling event (June 2005), indicating that groundwater flow within the study area is variable and may flow to the southeast during heavy precipitation events.

Data collected during the 12 months of the demonstration indicate that groundwater geochemistry within the biowalls has been modified to conditions conducive for anaerobic degradation processes to occur. Degradation of chlorinated ethenes has been stimulated through biologically mediated reductive dechlorination and biogeochemical reduction of PCE and TCE. However, significant reductions in total molar concentrations were not observed during the 12 month monitoring period.

Parsons recommended that the Air Force continue to monitor the biowall system on an occasional basis (perhaps every 1 to 2 years) to expand the understanding of the processes that are occurring within the biowalls and the long-term impacts the biowall system may have on groundwater quality.

1.3.3 Seneca Army Depot Activity

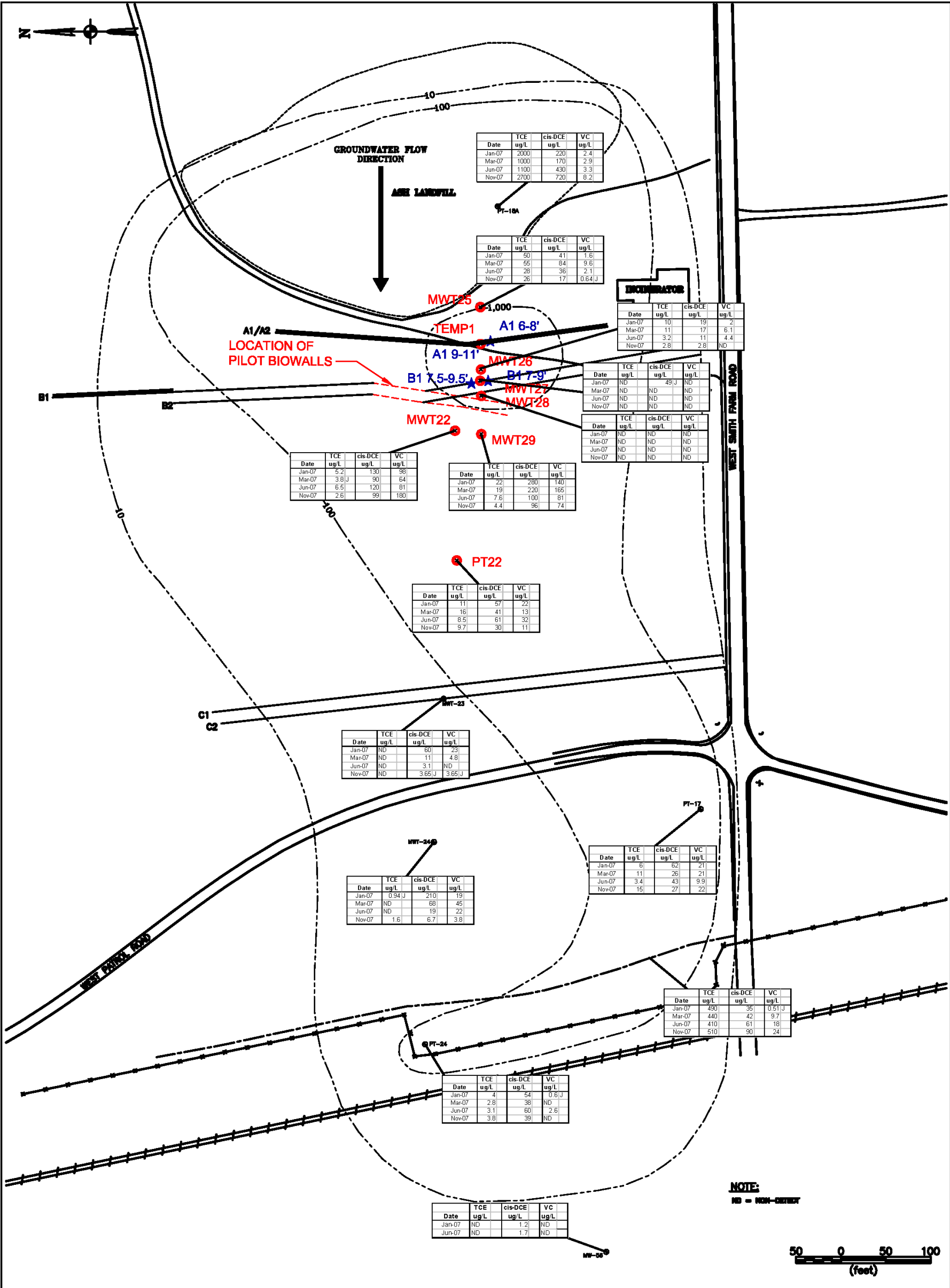
A permeable mulch biowall pilot test was used to enhance the *in situ* bioremediation of chlorinated solvents at the Ash Landfill at Seneca Army Depot Activity, Romulus, New York. Two parallel biowalls were installed in August 2005 as a dual biowall system, and five rounds of sampling were conducted in September 2005, October 2005, December 2005 and January 2006.

Based on pilot test results, the system has been expanded to full scale. The final full-scale design utilizes three sets of dual biowalls along the axis of the plume to reduce the overall time frame for remediation of the chlorinated ethene plume. Approximately 2,720 linear feet of biowalls has been installed, using approximately 6,240 cubic yards of a 50:50 mulch to sand mixture (by volume) coated with approximately 15,600 gallons of vegetable oil. A site map showing the full- and pilot-scale biowall locations, site features, and the monitoring network is provided in **Figure 1-4**. The full-scale system is currently being monitored on a quarterly basis. The historical data presented below are for the pilot test and not for the full-scale system that was sampled as part of this study.

Hydrogeology

Depth to groundwater within the pilot biowalls ranged from approximately 2.2 to 7.4 feet bgs during the pilot test. The biowalls were installed to the top of a competent shale (bedrock) surface. The depth of the eastern pilot trench averages 11.3 feet bgs and the depth of the western pilot trench is an average of 10.7 feet bgs. Therefore, the saturated thickness within the two biowall trenches ranges from 3.3 to 9.1 feet at any given time, depending on seasonal changes in groundwater levels due to recharge from precipitation.

The groundwater surface slopes northwest, with horizontal hydraulic gradients ranging from 0.02 ft/ft to 0.05 ft/ft. Hydraulic conductivity in the till/weathered shale formation ranges from 2.0×10^{-5} to 1.6×10^{-4} cm/sec. The hydraulic conductivity measured in the pilot biowalls were an order of magnitude greater, ranging from 1.0×10^{-3} to 7.3×10^{-3} cm/sec. Using the range of calculated hydraulic conductivity derived from slug test data, the range of horizontal hydraulic gradients, and an estimated effective porosity of 15 percent, the advective velocity of groundwater flow in the till/weathered shale formation ranges from approximately 0.010 to 0.14 ft/day (4.0 to 53 ft/yr).



LEGEND:

- PAVED ROAD
- DIRT ROAD
- RAILROAD TRACKS
- GROUNDWATER SAMPLING LOCATION
- BIOWALL MATERIAL SAMPLING LOCATION
- PILOT STUDY BIOWALL (2005)
- SINGLE BIOWALL (2006)
- DOUBLE-WIDE BIOWALL (2006)
- ZERO VALENT IRON WALL (1998)
- GROUNDWATER ISOCONTOUR (UG/L) BASED ON JANUARY 2000 DATA
- MONITORING WELL AND DESIGNATION
- CHAIN LINK FENCE

PARSONS

CLIENT/PROJECT TITLE
SENECA ARMY DEPOT
ASH LANDFILL
LONG-TERM MONITORING REPORT

DEPT. ENVIRONMENTAL ENGINEERING Dwg. No. 744538-01400

FIGURE 1-4
CHLORINATED ETHENES CONCENTRATIONS IN GROUNDWATER QTR 4 - NOVEMBER 2007

SCALE 1" = 100' DATE JANUARY 2006 REV -

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Observations of geochemical parameters monitored over the duration of the pilot test indicate that the groundwater advective velocity may be greater than aquifer (slug) test results indicate. Based on the time it took for breakthrough of geochemical parameters to be observed at the downgradient wells, it appears that flow through the North Transect may be on the order of 100 ft/yr, and flow through the South Transect may be between 200 and 400 ft/year. Based on these groundwater velocities, the residence time through the biowall system (approximately 18 feet) is approximately 66 days for the North Transect and between 16 and 33 days for the South Transect. Calculation of residence time does not account for the effects of a higher effective porosity with the biowall itself, nor do they account for sorption of contaminants onto the mulch matrix. Therefore, groundwater residence time calculations are considered conservative; actual contaminant residence time may be longer.

Historic System Performance

The primary contaminants detected at the site include TCE, *cis*-1,2-DCE, and VC. During the four sampling rounds, upgradient concentrations of TCE ranged from 400 µg/L to 860 µg/L, and upgradient concentrations of *cis*-1,2-DCE ranged from 310 µg/L to 980 µg/L. Concentrations of VC detected upgradient of the biowall system ranged from <1.2 µg/L to 24 µg/L in the South Transect (PT-12A), and from 64 µg/L to 86 µg/L in the North Transect (MWT-12R).

As of the second monitoring event in October 2005, a trend of decreasing TCE was observed at all monitoring locations within or downgradient of the biowall system. Concentrations of TCE continued to decrease even further from September to January 2006. In January 2006, concentrations of TCE have decreased to non-detect in the four monitoring wells located within the biowalls, and concentrations of TCE in the downgradient monitoring wells have been reduced to a range from 2.9 µg/L to 25 µg/L.

Concentrations of *cis*-1,2-DCE are reduced within each biowall, but rebound sharply between the two biowalls, particularly during the 13 week monitoring event. It is likely that at least a portion of the rebound in concentrations of *cis*-1,2-DCE between and downgradient of the biowalls is due to desorption of TCE and transformation to *cis*-1,2-DCE. Based on the fraction of organic carbon in the native sediments and the aqueous to organic carbon partitioning ratio of TCE, approximately 90 percent of the mass of TCE within the aquifer system is adsorbed to the aquifer matrix.

The reductions in total molar concentrations of chloroethenes within the biowalls relative to upgradient locations along the North and South Transects have ranged from approximately 86 to 99 percent over time. A reduction in total molar concentrations shows that the chlorinated ethenes are not simply being converted from one chlorinated ethene to another (i.e., accumulation of *cis*-1,2-DCE or VC), and that complete reduction to non-toxic degradation products is occurring. Total molar concentrations of chloroethenes are clearly depleted within the biowalls. A decrease in total molar concentrations is observed along the North Transect both within and downgradient of the biowall. An increase in total molar concentration downgradient of the biowalls may be due to 1) the continued desorption of TCE from native soils, 2) mixing with untreated groundwater, or 3) indicate that biodegradation may be limited to the immediate biowall reactive zone.

Geochemical Conditions

Comparison of geochemical parameters for biowall well locations MWT-13 and MWT-18 (East Biowall) and MWT-15 and MWT-20 (West Biowall) to well locations outside the biowall are summarized below.

- **Dissolved Oxygen.** Dissolved oxygen levels were already naturally depleted, being less than 2.0 mg/L in the study area. In the last round of sampling (January, 2006), concentrations of dissolved oxygen were less than 0.30 mg/L at all sample locations up to 150 feet downgradient of the biowalls.
- **Oxidation-Reduction Potential.** Through the first two rounds of sampling, the oxidation-reduction potential upgradient of the biowall has ranged from +214 mV to +304 mV, indicating background conditions are only mildly anoxic. Within the East and West Pilot Biowalls, the oxidation-reduction potential has been lowered to a range of +67 mV to -16 mV. By January 2006, all monitoring locations downgradient of the biowalls (to a distance of 22.5 feet) exhibited an oxidation-reduction potential less than -100 mV, indicating that highly reducing conditions are present over a large area downgradient of both pilot biowalls.
- **Ferrous Iron.** Concentrations of Fe+2 upgradient of the biowall are less than 0.5 mg/L. Within the biowall, concentrations of Fe+2 are elevated, with a maximum concentration of 5.1 mg/L measured at location MWT-15 in October 2005. Elevated concentrations of Fe+2 were observed in downgradient locations, although elevated concentrations were not evident in PT-22, located 150 feet downgradient of the biowalls.
- **Sulfate.** Sulfate levels upgradient of the biowalls during the pilot test ranged from 325 to 903 mg/L. By the second round of sampling, the levels of sulfate were depleted to non-detect levels within the biowalls, except for the January 2006 round in MWT-15 (33 mg/L).
- **Methane.** Methane concentrations in the two upgradient wells range from 0.001 mg/L to 0.15 mg/L. Concentrations of methane measured in the biowalls were elevated at 3.1 mg/L to 8.1 mg/L in September 2005, and increased to 14 mg/L to 28 mg/L in January 2006.
- Overall, highly anaerobic conditions were stimulated within and immediately downgradient of the pilot biowalls. Predominant terminal electron accepting processes are iron reduction, sulfate reduction, and methanogenesis.
- Reductions in the concentration of TCE between the upgradient wells and the wells within the second biowall (West Biowall) are greater than 99 percent.
- Reductions in total molar chlorinated ethenes between the upgradient wells and the wells within the second biowall (West Biowall) are between 86 percent and 99 percent.
- Geochemical data and reductions in chlorinated ethenes indicates that treatment zones have been readily established within and downgradient of the dual biowall system. Development of the treatment zone along the South Transect, although present, appears to lag development along the North Transect by about 40 to 50 days.

- The molar fraction of ethene is increasing within and downgradient of the biowall system and is a positive indicator of complete biotic dechlorination of chlorinated ethenes at the site.
- Sufficient performance design information acquired during the pilot test led to the design and installation of a full-scale biowall.

The biowall performance at the Seneca Army Depot Activity was shown to be comparable to, and in some cases better than, that of a zero-valent iron wall at the site during its first year of performance. Based on the performance and cost of the pilot biowall system relative to the pilot-scale zero-valent iron wall, a full-scale biowall system was selected as the final remedy for the Ash Landfill site to prevent off-Depot migration of chlorinated ethenes and to reduce the overall time for site cleanup.

1.3.4 Dugway Proving Ground

A pilot test was conducted at Dugway Proving Ground SWMU-97 site that involved injection of emulsified vegetable oil. Thus the evaluation of *in situ* biogeochemical transformation at Dugway Proving Ground differs from the other sites in that a liquid electron donor was injected into the aquifer rather than installation of a biowall.

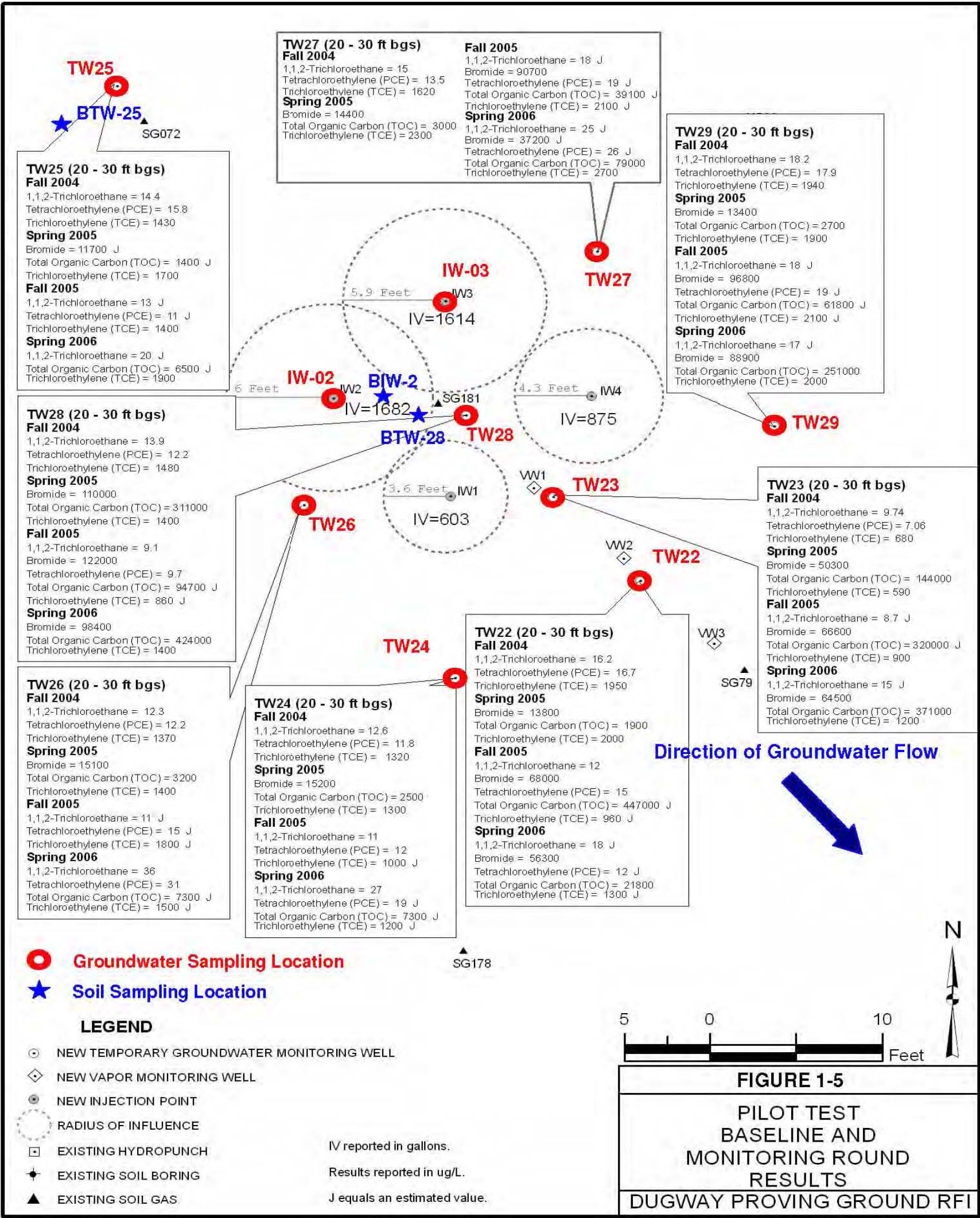
Four injection points were installed on approximately 10-foot centers, screened from 20 to 30 feet bgs. Eight performance monitoring points were installed, screened from 20 to 30 feet bgs. Four monitoring events have been conducted from November 2004 to April 2006. A field mixed emulsion was injected in November 2004, with approximately 3,000 pounds of vegetable oil emulsified with lecithin and site groundwater. **Figure 1-5** provides a map showing the site features, the injection well location and the monitoring network.

Hydrogeology

The subsurface at Dugway Proving Ground site is characterized by four clay strata labeled Clay 1 through Clay 4, interspersed with four water bearing strata labeled Sand A through Sand D. Underlying Sand D is an aquitard, and beneath that is a deep potable aquifer. Sand A and Clay B are poorly developed. Sand B is the horizon targeted for treatment. Sand B runs 18 to 21 feet thick, with the top of Sand B at approximately 22 feet bgs.

Groundwater flow is from the northwest to the southeast along the longitudinal axis of the chlorinated ethene plume. The hydraulic conductivity in Sand B has been estimated at 2.62×10^{-3} cm/sec. Boring logs indicate that significant heterogeneity exists in the composition of Sand B. Based on piezometer results and boring logs, the upper 10 feet of Sand B are more sandy than the lower 10 feet of the unit, which are significantly more silty.

On the longitudinal axis of the plume, the groundwater flow rate is estimated at 35 ft/yr, based on BIOCHLOR modeling. Given the uncertainties in hydraulic conductivity and plume age, which were used to obtain this value, it should be noted that actual groundwater velocities may differ significantly from this value.



Historic System Performance

Concentrations of TCE at the site ranged from 590 µg/L at location TW23 in November 2005, up to 2,700 µg/L at location TW27 in April 2006. There were no apparent trends over time in the concentration of TCE. Lower concentrations of PCE were observed (< 30 µg/L).

Concentrations of *cis*-1,2-DCE were generally non-detect, remaining less than 10 µg/L for the duration of the pilot test. VC was not detected at any sample location.

Given the lack of any decreasing trend in TCE, and a lack of production of *cis*-1,2-DCE or VC, it appears that neither biotic reductive dechlorination or biogeochemical reduction have been stimulated at the Dugway Proving Ground site. It is possible that the high total dissolved solids (i.e., 60,000 mg/L including 10,400 mg/L sulfate) at this site may be inhibitory to some anaerobic degradation processes.

Geochemical Conditions

Comparison of geochemical parameters for upgradient well location TW-25 to well locations within the injection area (e.g., TW23 and TW28) are summarized below.

- **Total Organic Carbon.** Concentrations of total organic carbon in upgradient location TW25 remained less than 10 mg/L during the pilot test. At wells TW23 and TW28, located within the injection area, total organic carbon ranged from 95 mg/L (estimated concentration) up to 424 mg/L after injection. The highest levels of total organic carbon at these locations were observed during the last sampling round in April 2006, indicating that substrate levels were not depleted over the 17 months of monitoring following injection.
- **Dissolved Oxygen.** Dissolved oxygen levels are naturally depleted, being less than 2.0 mg/L in the study area.
- **Oxidation-Reduction Potential.** The oxidation-reduction potential upgradient of the injection area has ranged from +340 mV to +89 mV, gradually becoming more negative over time and indicating background conditions are mildly anoxic. Within the injection area at wells TW23 and TW28, the oxidation-reduction potential has been lowered to a range of +55 mV to -36 mV after injection. This range of oxidation-reduction potentials appears sufficient to support iron and sulfate reduction.
- **Ferrous Iron.** Concentrations of Fe⁺² upgradient of the biowall are less than 0.05 mg/L. Within the injection zone at wells TW23 and TW28, concentrations of Fe⁺² ranged from 2.3 to 11 mg/L after injection. Elevated concentrations of Fe⁺² were observed in down gradient locations TW22 and TW29, and in cross gradient location TW29.
- **Sulfate and Sulfide.** Sulfate levels upgradient of the biowalls during the pilot test ranged from 10,900 to 12,000 mg/L. Within the injection area (TW23 and TW28), the concentration of sulfate was only slightly depleted, ranging from 10,000 to 11,000 mg/L after injection. Hydrogen sulfide levels were generally elevated where elevated levels of total organic carbon were observed. Background levels of hydrogen sulfide were less than 0.01 mg/L, while the highest concentration of hydrogen sulfide measured was 1.3 mg/L at TW28 in November 2005.
- **Methane.** Methane concentrations within the injection area remained less than 0.05 mg/L

during the pilot test, indicating methanogenesis is not a significant terminal electron accepting process at this site.

- Total Dissolved Solids. One important characteristic of groundwater at the Dugway Proving Ground site is high total dissolved solids levels. In general, the total dissolved solids ranges from 41,000 to 59,000 mg/L, while chloride ranges from 21,000 to 29,000 mg/L. It is not known what inhibitory effects high total dissolved solids may have on anaerobic degradation processes at this site.

Overall, anaerobic conditions at the Dugway Proving Ground site were stimulated within and immediately downgradient of the pilot test injection area. Predominant terminal electron accepting processes are iron reduction and sulfate reduction, but methanogenesis was not evident.

Given the lack of any decreasing trend in TCE, and a lack of production of *cis*-1,2-DCE or VC, it is apparent that neither biotic reductive dechlorination or biogeochemical reduction have been stimulated at the Dugway Proving Ground site. It is possible that the high total dissolved solids at this site may inhibit some anaerobic degradation processes. However, ferrous iron and sulfide data suggests that iron and sulfate reduction have been stimulated. Field crews report a strong hydrogen sulfide (rotten egg) odor from groundwater samples. It is likely that iron sulfide minerals have been precipitated, but it is unknown why biogeochemical reduction of TCE is not apparent.

2.0 Sampling and Analysis

2.1 Sampling

Sampling activities associated with this project included collecting biowall material and groundwater for biowall applications at Altus AFB, Oklahoma; Dover AFB, Delaware; and Seneca Army Depot Activity, New York. Field activities at the Dugway Proving Ground, Utah included sampling of soil and groundwater for an application of emulsified vegetable oil. This section describes the sampling activities, locations, sample protocols, and sampling methods followed at each site. Field sampling methods are described in the project Field Sampling Plan (FSP) (Parsons, 2008), while the analyses performed on the samples are discussed in Section 2.2.

There were exceptions to following the FSP. Sampling at the Altus AFB sites were not collected in accordance with the Parsons FSP, as the sampling and analysis was conducted by the USEPA NRMRL/GWERD. In addition, groundwater sampling conducted at Seneca Army Depot Activity by Parsons for the United States Army Corps of Engineers (USACE) followed quality assurance/quality control (QA/QC) procedures for that program. Although there were some differences in the USEPA NRMRL/GWERD, USACE, and Parsons procedures, sample collection and handling methods were very similar and are summarized in the following sections.

2.1.1 Soil and Biowall Sampling Procedures

Soil and biowall samples were collected using both direct-push and auger drilling techniques. Because these samples contained reduced iron and sulfide minerals that are vulnerable to oxidation by exposure to the atmosphere, they required special handling and preservation. The following is the sampling protocol followed for collection of these samples.

2.1.1.1 Borehole Advancement

During borehole advancement, biowall or soil samples were collected for visual description. Biowall material samples were collected using a specialized direct-push method to collect samples frozen *in situ*. Soil samples at Dugway Proving Ground were collected using a standard split-spoon sampler with clear polyvinyl chloride (PVC) liners. At each borehole location, one or more biowall material or soil samples were collected from the saturated zone. The soil or biowall cuttings were handled in accordance with the investigation-derived waste (IDW) procedures discussed for each of the sites.

A field scientist was responsible for maintaining a descriptive log of subsurface materials recovered during drilling, recording field measurements, collecting biowall or soil samples, and properly labeling and storing samples. A boring log was prepared for each soil boring. The log described the sample intervals, lithology, presence or absence of signs of contamination, and any other pertinent observations. Boring logs were not prepared for sampling of biowall materials due to the uniformity of the backfill mixtures.

2.1.1.2 Soil Sampling Procedure for Direct-Push Using Core Barrels with Liners

Procedures used to collect soil samples using the direct-push technology (Dugway Proving Ground) were as follows:

- Collect the soil sample in a clear PVC liner contained within a split barrel sampler. The liners had an inner diameter of 2 inches and were 5 feet long.
- Retrieve the sample and identify the appropriate sample interval based on presence of black mineral staining (sulfides).
- Cut the section of the core sleeve containing the soil sample to a length of 12 inches and cap immediately.
- Label the sample then seal in two nested Zip Lock™ bags, tape the bags, and place in cooler with dry ice to freeze.

Samples were packed in a cooler with dry ice and remained frozen until delivered to the laboratory. Samples were shipped overnight via FedEx to the USEPA NRMRL/GWERD in Ada, Oklahoma.

2.1.1.3 Sampling Procedure for *In Situ* Frozen Biowall Samples

A specialized procedure was developed by USEPA to collect *in situ* frozen biowall samples to minimize oxidation upon exposure to air. The specialized equipment and procedure for collecting *in situ* frozen biowall material samples at Altus AFB, Seneca Army Depot Activity, and Dover AFB are summarized below.

Equipment

- One-inch inside-diameter steel direct-push rods with a fixed, solid drive tip. The drive tip has a diameter slightly larger than the drive rod outside diameter to create a shoulder to retain the frozen samples.
- 1/4- or 3/8-inch diameter copper tubing.

- Liquid nitrogen “sprayer” consisting of an 18-inch length of the above copper tubing with the bottom end crimped closed, the top fitted with a standard compression fitting, and 1/16- to 3/32-inch holes drilled along the length.
- Liquid nitrogen in a pressurized, bottom-discharge, cryogenic liquid container (Dewar). Cryogenic hose with fittings to connect the nitrogen Dewar to the copper tubing.
- Approximately 15 to 20 liters of liquid nitrogen is required per sample.
- Specialized personal protective equipment (PPE, e.g., gloves and face shields) for handling cryogenic media.

Sampling Procedure

- Drill through the soil overburden to approximately one foot above the top of the desired sample interval with 6-inch inside-diameter hollow stem augers. Retract the inner drill string.
- Push the steel direct-push drive rod past the bottom of the auger flights to the bottom of the desired sample interval.
- Attach the nitrogen sprayer to the copper tubing and insert the sprayer to the bottom of the push-rods.
- Apply liquid nitrogen for approximately 5 to 10 minutes to create an approximately 2-inch thick layer of frozen biowall material on the outside of the lead drive rod.
- Stop the flow of nitrogen then immediately withdraw the drive rods with the frozen sample attached to the rods.
- Place the push rod with sample on a clean plastic sheet and remove the desired sample interval using a decontaminated rock hammer.
- Immediately place the frozen sample into a Zip Lock™ bag, attach the sample label with clear tape, seal the sample in a second Zip Lock™ bag, then place on dry ice to maintain the sample in a frozen state.

Samples were packed in a cooler with dry ice and remained frozen until delivered to the laboratory. Samples were shipped overnight via FedEx to the USEPA NRMRL/GWERD in Ada, Oklahoma.

2.1.2 Groundwater Sampling

2.1.2.1 Purging and Sample Collection

All equipment and meters used for purging and sampling was properly cleaned and calibrated (if required) according to the manufacturers’ specifications prior to field use. Prior to removing any water from the sampling well, the static water level and total well depth were measured using an electric water-level probe. Disposable tubing was used to purge and sample the wells.

Prior to sampling, the monitoring wells were purged using a peristaltic pump and the micropurging method. The pump intake was positioned at the approximate mid-point of the saturated screened interval. Purging continued until a minimum 3 casing volumes of water had been removed from the well and until pH, temperature, specific conductance, dissolved oxygen,

and oxidation-reduction potential stabilized. Purge water was collected and disposed of according to the IDW procedures described for each site.

Samples were collected after stable conditions were achieved. A peristaltic pump was used to extract groundwater for the sample. The extracted groundwater was transferred directly into the appropriate sample containers provided by the laboratories. The water was carefully poured down the inner walls of the sample container to minimize aeration of the sample.

An exception was made for Dugway Proving Ground where a submersible pump (Grunfos® Brand) was used for purging the wells. After purging, sampling was conducted with a peristaltic pump as described above.

2.1.2.2 Sampling Activities at Altus AFB, Oklahoma

Sampling activities at the OU-1 and SS-17 biowall sites at Altus AFB, Oklahoma consisted of sampling biowall materials and groundwater. Sampling locations for OU-1 are identified on **Figure 1-1** and sampling locations for the B Transects at SS-17 are identified on **Figure 1-2**. The well transects targeted for evaluation are the Northern Transect at OU-1 and the B4 and B5 Transects at SS-17.

Altus AFB Biowall Material Sampling

Biowall material samples were collected at the OU-1 Northern Transect by the USEPA NRMRL/GWERD on September 6, 2007. Six samples of biowall material were collected from the saturated portion of the OU-1 biowall adjacent to monitoring well MP1, installed within the biowall trench. Samples were collected at depths ranging from 5.0 to 20.5 feet bgs. Three biowall material samples were also collected at the SS-17 Section B biowall, Well Transect B4, adjacent to well BB04W. Samples from biowall at the B4 Transect were collected at depths ranging from 6.0 to 19.5 feet bgs.

Altus AFB Groundwater Sampling

Sampling was conducted at the five monitoring wells at OU-1 and six wells at SS17 Sites as shown on **Figures 1-1** and **1-2**. Sampling was performed for this investigation on September 6, 2007.

2.1.2.3 Sampling Activities at Dover AFB, Delaware

Sampling activities at the WP-14 biowall site at Dover AFB, Delaware included sampling of biowall materials and groundwater from 17 to 20 March 2008. Sampling locations are identified on **Figure 1-3**. Two well transects were targeted for evaluation, the Northern Transect and the Southern Transect. These transects are oriented along flow paths through both the east (upgradient) and west (downgradient) biowalls. Biowall material was collected from both biowalls.

Sampling of Biowall Material – Dover AFB

Samples of biowall backfill material were collected from the biowalls adjacent to wells TS-MW01 and TS-MW-03 (Northern Transect), and adjacent to wells TS-MW06 and TS-MW08 (Southern Transect). Two samples of biowall material from each location were collected from

the saturated portion of the biowalls adjacent to existing monitoring wells installed within the biowall trench. Samples were collected from approximately 10 to 19 feet bgs.

Groundwater Sampling – Dover AFB

Groundwater sampling was conducted at 10 monitoring wells shown on **Figure 1-3**.

2.1.2.4 Sampling Activities at Seneca Army Depot Activity

Sampling activities at the Ash Landfill biowall site at Seneca Army Depot Activity, New York included sampling of biowall materials and groundwater at the A1 and B1/B2 biowalls.

Sampling locations are identified on **Figure 1-4**. An extended well transect from upgradient of the first biowall section (A1) through the second set of biowalls (B1/B2) was targeted for evaluation. These transects are oriented along flow paths through the A1 (upgradient) and B1/B2 (downgradient) biowalls.

Biowall Materials Sampling – Seneca Army Depot Activity

Two biowall material samples were collected from a temporary boring location (TEMP-1) in the A1 biowall. One biowall mulch sample was collected from each of two borings in the B1 biowall adjacent to existing well MWT-27. Two borings were required in the B1 biowall because bedrock was encountered at a depth shallower than expected in the first boring and a deeper sample could not be collected. Therefore, an additional sample was collected from a second adjacent borehole. Samples were collected from approximately 6 to 11 feet bgs.

The biowall material samples were sent to the USEPA NRMRL/GWERD in Ada, Oklahoma.

Groundwater Sampling – Seneca Army Depot Activity

Fourteen wells were sampled as part of monitoring the biowall remedy at the Ash Landfill Site. Data collected in November 2007 by Parsons for Seneca Army Depot Activity was used for this project. Supplemental groundwater sampling was conducted under this project from January 8 to 10, 2008 at eight monitoring well locations.

2.1.2.5 Sampling Activities at Dugway Proving Ground, Utah

Sampling activities at the SWMU-97 pilot test site at Dugway Proving Ground, Utah included soil and groundwater sampling. Sampling locations are identified on **Figure 1-5**. Soil and groundwater samples were collected within and upgradient of the reaction zone created by the injection of emulsified vegetable oil.

Soil Sampling – Dugway Proving Ground

Soil samples were collected using a 5-foot long by 2-inch diameter split-spoon sampler fitted with clear PVC liners. After retrieving the samples, they were immediately frozen on dry ice and then maintained in a frozen state until received by the laboratory.

Soil samples were collected from two locations within the vegetable oil injection area, adjacent to wells IW-02 (BIW2) and TW28 (BTW28). In addition, a soil sample was collected from a location upgradient from the injection area, adjacent to well TW25 (BTW25), to provide data for natural background conditions. Soil samples from borings within the injection area were collected from intervals with black, stained soil within the saturated zone. Two soil samples,

plus one field duplicate, were collected from BTW28. Three samples were collected from BIW2. Although the work plan specified collecting two samples from each boring in the injection zone, three samples were collected from BIW2 because of the zone of stained soil extended over a greater depth interval than anticipated. Samples at all locations were collected between approximately 14 and 26 feet bgs.

Groundwater Sampling – Dugway Proving Ground

Groundwater sampling was conducted at 10 monitoring wells at the SWMU-97 site, as shown on **Figure 1-5**, on April 22 to 24, 2008.

2.2 Analytical Procedures

A summary of the analyses performed for each site is presented in **Tables 2-1** through **2-4**, while a summary of the techniques used is presented in the following sections. All laboratory results for soil and water are presented in Appendices A and B, respectively.

**Table 2-1 - Summary of Sampling Activities at SS-17 and OU-1 Biowalls
Altus AFB, Oklahoma**

Location Identifier	Location Relative to Biowall	Water Level Measurement	Solid Sample Analyses			Groundwater Analyses								
			Mineral Extraction	Electron Microprobe	Total Organic Carbon	VOCs ^b	MEEA ^c	Dissolved Inorganics Cations	Dissolved Inorganics Anions	Stable Carbon Isotopes (Microseeps SOP)	Organic Carbon ^d	Total Dissolved Solids (SM 2540C)	Well Head Analyses ^e	Mobile Lab Analyses ^f
			Protocol ^a	Analysis	(SW9060M)									
			(USEPA)	(CU)	(CDM)	(USEPA)	(USEPA)	(USEPA)	(USEPA)	(MS)	(USEPA)	(USEPA)	(Field)	(Field)
Transect B4, SS-17														
BB04U	30' Upgradient	1				1	1	1	1	1	1	1	1	1
BB04W	Within Biowall	1	3	3	3	1	1	1	1	1	1	1	1	1
BB04D	30' Downgradient	1				1	1	1	1	1	1	1	1	1
Transect B5, SS-17														
BB05U	30' Upgradient	1				1	1	1	1	1	1	1	1	1
BB05W	Within Biowall	1				1	1	1	1	1	1	1	1	1
BB05D	30' Downgradient	1				1	1	1	1	1	1	1	1	1
Northern Transect, OU-1														
EPAUMP1	30' Upgradient	1				1	1	1	1	1	1	1	1	1
MP01	Within Biowall	1	6	6	6	1	1	1	1	1	1	1	1	1
MP02	5' Downgradient	1				1	1	1	1	1	1	1	1	1
MP03	10' Downgradient	1				1	1	1	1	1	1	1	1	1
MP04	30' Downgradient	1				1	1	1	1	1	1	1	1	1
SUBTOTALS		11	9	9	9	11	11	11	11	11	11	11	11	11
QA/QC														
Duplicates			2	1	1	1	1	1	1		1	1		
MS						1								
MSD						1								
Trip Blanks														
TASK TOTAL		11	11	10	10	14	12	12	12	11	12	12	11	11

Notes:

Samples at Altus AFB were collected by the USEPA NRMRL/GWERD in September 2007.

Analyses performed by USEPA = USEPA NRMRL; CU = University of Colorado; CDM = Camp Dresser & McKee Inc.; MS = Microseeps, Inc.; Field = field analysis using direct-reading meters and Hach Company test methods.

a) Biowall material protocol includes iron and sulfide extractions.

b) VOCs - volatile organic compounds.

c) MEEA - Methane, ethane, ethene, and acetylene.

d) Organic carbon analyses included total organic carbon, dissolved organic carbon, dissolved inorganic carbon, and total carbon.

e) Well head analyses included dissolved oxygen, oxidation-reduction potential, pH, temperature, and conductivity.

f) Mobile lab analyses included alkalinity, ferrous iron, and sulfide.

Table 2-2 - Summary of Sampling Activities at Site WP-14
Dover AFB, Delaware

Location Identifier	Location	Water	Solid Sample Analyses			Groundwater Analyses										
			Mineral	Electron	Total	VOCs ^b	MEEA ^c (AM20 GAX)	Dissolved	Dissolved	Stable	Dissolved	Nitrate +	Sulfide	Total	Well	Mobile
			Extraction	Microprobe	Organic			Inorganics	Inorganics	Carbon	Organic	Nitrite		Dissolved	Head	Lab
			Protocol ^a	Analysis	Carbon			Cations	Anions	Isotopes	Carbon	Nitrite		Solids	Analyses ^d	Analyses ^e
	Relative to Biowall	Level Measurement	(USEPA)	(CU)	(CDM)	(MS)	(MS)	(MS)	(MS)	(MS)	(MS)	(MS)	(MS)	(MS)	(Field)	(Field)
Northern Transect																
TS-MW11	Upgradient	1				1	1	1	1	1	1	1	1	1	1	1
TS-MW01	Within First Biowall	1	2	2	2	1	1	1	1	1	1	1	1	1	1	1
TS-MW02	Between Biowalls	1				1	1	1	1	1	1	1	1	1	1	1
TS-MW03	Within Second Biowall	1	2	2	2	1	1	1	1	1	1	1	1	1	1	1
TS-MW04	Downgradient	1				1	1	1	1	1	1	1	1	1	1	1
TS-MW05	Downgradient	1														
Southern Transect (Sulfate Added)																
TS-MW12	Upgradient	1				1	1	1	1	1	1	1	1	1	1	1
TS-MW06	Within First Biowall	1	2	2	2	1	1	1	1	1	1	1	1	1	1	1
TS-MW07	Between Biowalls	1				1	1	1	1	1	1	1	1	1	1	1
TS-MW08	Within Second Biowall	1	2	2	2	1	1	1	1	1	1	1	1	1	1	1
TS-MW09	Downgradient	1				1	1	1	1	1	1	1	1	1	1	1
TS-MW10	Downgradient	1														
Site Monitoring Wells																
MW011	Upgradient	1														
MW012	Upgradient	1														
MW013	Upgradient	1														
GSCP9A,B,S	Upgradient	3														
SUBTOTALS		12	8	8	8	10	10	10	10	10	10	10	10	10	10	10
QA/QC																
Duplicates			1	1	1	1	1	1	1	1	1	1	1	1	1	1
MS						1										
MSD						1										
Trip Blanks						1										
TASK TOTAL		12	9	9	9	14	11	11	11	11	11	11	11	11	11	11

Notes:

Analyses were performed by USEPA = USEPA NRMRL/GWERD; CU = University of Colorado; CDM = Camp Dresser & McKee Inc.; MS = Microseeps, Inc.; Field = field analysis using meters and Hach Company test methods.

- a) Biowall material protocol included iron and sulfide extractions.
- b) VOCs - volatile organic compounds.
- c) MEEA - methane, ethane, ethene, and acetylene.
- d) Well head analyses include dissolved oxygen, oxidation-reduction potential, pH, temperature, and conductivity.
- e) Mobile lab analyses include alkalinity, carbon dioxide, ferrous iron, manganese, and hydrogen sulfide.

**Table 2-3 - Summary of Sampling Activities at the Ash Landfill Site
Seneca Army Depot Activity, New York**

Location Identifier	Location Relative to Biowall	Water Level Measurement	Solid Sample Analyses			Groundwater Analyses									
			Mineral Extraction Protocol ^a (USEPA)	Electron Microprobe Analysis (CU)	Total Organic Carbon (SW9060M) (CDM)	VOCs ^b (SW8260B) (TA)	MEE ^c (AM20 GAX) (MS)	Dissolved Inorganics Cations (SW6010B) (MS)	Dissolved Inorganics Anions (SW9056) (MS)	Stable Carbon Isotopes (Lab SOP) (MS)	Dissolved Organic Carbon (SW9060) (TA)	Nitrate + Nitrite (E353.3) (MS)	Total Dissolved Solids (E160.1) (MS)	Well Head Analyses ^d (Field)	Mobile Lab Analyses ^e (Field)
PT-18	Upgradient in Landfill	1				X								X	
MWT-25	Upgradient A1/A2	1				X		1	1	1		1	1	X	
TEMP-1 (abandoned)	Within A1/A2 Biowall		2	2	2	1	1	1	1	1	1	1	1	1	1
MWT-26	Upgradient B1/B2 Biowall	1				X	X	1	1	1	X	1	1	X	X
MWT-27	Within B1 Biowall	1	2	2	2	X	X	1	1	1	X	1	1	X	X
MWT-28	Within B2 Biowall	1				X	X	1	1	1	X	1	1	X	X
MWT-29	Downgradient B1/B2	1				X	X	1	1	1	X	1	1	X	X
MWT-22	Downgradient B1/B2	1				X		1	1	1		1	1	X	
PT-22	Downgradient B1/B2	1				X		1	1	1		1	1	X	
MWT-23	Within C2 Biowall	1				X	X				X			X	X
MWT-24	Downgradient C1/C2 Biowall	1				X								X	
PT-17	Downgradient C1/C2 Biowall	1				X								X	
MWT-7	Downgradient C1/C2 Biowall	1				X								X	
PT-24	Downgradient C1/C2 Biowall	1				X								X	
MW-56	Off-Site					X								X	
SUBTOTALS		8	4	4	4	1	1	8	8	8	1	8	8	1	1
QA/QC															
Duplicates						1	X	1	1	1	X	X	1	X	X
MS						X									
MSD						X									
Trip Blanks						1									
TASK TOTAL		8	4	4	4	3	1	9	9	9	1	8	9	1	1

Notes:
Analyses were performed by USEPA = USEPA NRMRL/GWERD Lab; CU = University of Colorado; CDM = Camp Dresser & McKee Inc.; TA = Test America; MS = Microseeps, Inc.; Field = field analysis using meters and Hach Company test methods.
"X" indicates a sample that was collected and analyzed by Parsons under the remediation monitoring plan for this site.
a) Biowall material protocol included iron and sulfide extractions.
b) VOCs - volatile organic compounds.
c) MEEA - methane, ethane, and ethene.
d) Well head analyses include dissolved oxygen, oxidation-reduction potential, pH, temperature, and conductivity.
e) Mobile lab analyses included ferrous iron and manganese.

Table 2-4 - Summary of Sampling Activities at SWMU-97
Dugway Proving Ground, Utah

Location Identifier	Location Relative to Reaction Zone	Water Level Measurement	Solid Sample Analyses			Groundwater Analyses														
			Mineral Extraction	Electron Microprobe	Total Organic Carbon	VOCs ^b	MEEA ^c (AM20 GAX)	Dissolved Inorganics Cations	Dissolved Inorganics Anions	Chloride, Nitrate, Sulfate, Bromide	Stable Carbon Isotopes (Lab SOP)	Dissolved Organic Carbon	Volatile Fatty Acids (Lab SOP)	Phospholipid Fatty Acids (Lab SOP)	Quantitative PCR for <i>Dehalococcoides</i> (Lab SOP)	Dissolved Metals (SW6010)	Total Dissolved Solids (E160.1)	Sulfide (SM4500)	Well Head Analyses ^d	Mobile Lab Analyses ^e
			Protocol ^a (USEPA)	Analysis (CU)	(SW9060M) (CDM)	(SW8260B) (TA)	(MS)	(SW6010B) (TA,MS)	(SW9056) (TA,MS)	(SW9056) (TA)	(MS)	(TA)	(MS)	(MI)	(MI)	(TA)	(MS)	(MS)	(Field)	(Field)
TW-22	Downgradient	1				1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TW-23	Downgradient	1				1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TW-24	Downgradient	1				1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TW-25	Upgradient	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TW-26	Crossgradient	1				1	1	1	1	1		1	1	1	1	1			1	1
TW-27	Crossgradient	1				1	1	1	1	1		1	1	1	1	1			1	1
TW-28	Within Injection Area	1	2	2	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
TW-29	Down/Crossgradient	1				1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
IW-1	Injection Well	1																		
IW-2	Injection Well	1	3	3	3	1	1	1	1	1	1	1					1	1	1	1
IW-3	Injection Well	1				1	1	1	1	1	1	1					1	1	1	1
IW-4	Injection Well	1																		
SUBTOTALS		12	6	6	6	10	10	10	10	10	8	10	8	8	8	8	8	8	10	10
QA/QC																				
Duplicates			1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
MS						1	1			1		1	1	1	1	1				
MSD						1	1			1		1	1	1	1	1				
Trip Blanks						2														
TASK TOTAL		12	7	7	7	15	13	11	11	13	9	13	11	11	11	11	9	9	11	11

Notes:

Analyses were performed by USEPA = USEPA NRMRL/GWERD Lab; CU = University of Colorado; CDM = Camp Dresser & McKee Inc.; TA = Test America; MS = Microseeps, Inc.; MI = Microbial Insights; Field = field analysis using meters and Hach Company test methods.

a) Soil protocol included iron and sulfide extractions.

b) VOCs - volatile organic compounds.

c) MEEA - methane, ethane, ethene, and acetylene.

d) Well head analyses include dissolved oxygen, oxidation-reduction potential, pH, temperature, and conductivity.

e) Mobile lab analyses included alkalinity, carbon dioxide, ferrous iron, manganese, and hydrogen sulfide.

2.2.1 Biowall Mulch and Aquifer Matrix Analyses

A summary of the biowall/aquifer matrix sampling locations is shown in **Table 2-5** below.

Table 2-5- Summary of Biowall/Reaction Zone Samples

Description	Sample Identification	Description
Altus AFB, OU-1 Site	EPA-C1-A	2 ft north of well MP6 (OU-1 site, 9.0-10.5 ft depth)
	EPA-C3-A	5 ft north of well MP1 (OU-1 site, 5.0-6.5 ft depth)
	EPA-C4-A	5 ft north of well MP1 (OU-1 site, 6.5-8.0 ft depth)
	EPA-C5-A	5 ft north of well MP1 (OU-1 site, 11.5-13 ft depth)
	EPA-C6-A	5 ft north of well MP1 (OU-1 site, 16-17.5 ft depth)
	EPA-C7-A	5 ft north of well MP1 (OU-1 site, 19-20.5 ft depth)
Altus AFB, SS-17 Site	EPA-C11-A	5 ft east of BB04W (SS-17 site, 6-7.5 ft depth)
	EPA-C13-A	5 ft east of BB04W (SS-17 site, 12-13.5 ft depth)
	EPA-C15-A	5 ft east of BB04W (SS-17 site, 18-19.5 ft depth)
USEPA Column (Altus AFB SS-17 + hematite)	B3 1-1	Slice 1, 5 cm from inlet, see He et al. (2008)
	B3 3-1	Slice 3, 15 cm from inlet
	B3 5-1	Slice 5, 25 cm from inlet
	B3 7-1	Slice 7, 35 cm from inlet
Dover AFB	DTSB-1-10	Upgradient wall – South transect (10 ft depth)
	DTSB-1-17	Upgradient wall – South transect (17 ft depth)
	DTSB-3-10	Downgradient wall – South transect (10 ft depth)
	DTSB-3-16	Downgradient wall – South transect (16 ft depth)
	DTSB-6-10	Upgradient wall – North transect (10 ft depth)
	DTSB-8-10	Downgradient wall – North transect (10 ft depth)
	DTSB-8-17	Downgradient wall – North transect (17 ft depth)
	UTSB-16-10	Duplicate of DTSB-6-10
Seneca Army Depot Activity Wall A (upgradient)	SA1-9-11	Wall A1 (9-11 ft depth)
	SA1-6-8	Wall A1 (6-8 ft depth)
Seneca Army Depot Activity Wall B (downgradient)	SB1-7-9	Wall B1 (south of well MWT-27, 7-9 ft depth)
	SB1-7.5-9.5	Wall B1 (north of well MWT-27, 7-9.5 ft depth)
Dugway Proving Ground	97S-0086	Borehole TW-25, 23.8-25 ft depth (upgradient)
	97S-0087	Borehole TW-28, 24.75-26 ft depth (injection zone)
	97S-0088	Borehole IW-2, 22-23 ft depth (upgradient)
	97S-0089	Borehole IW-2, 24-25 ft depth (upgradient)
	97S-0090	Borehole TW-28, 21-22.5 ft depth (injection zone)
	97FD-0090	Borehole TW-28, 21-22.5 ft depth (duplicate of 97S-0090)
	97S-0091	Borehole BIW2, 14-15.25 ft depth (upgradient)

2.2.1.1 Electron Microprobe (EMP)

Analyses on a single grain of sediment or mulch were accomplished using an electron microprobe. Not only can analyses be performed on particles as small as one micron, but the electron microprobe also provides a visual picture of the soil at magnifications ranging from 40 to 300,000 times. The visual mode is referred to as the "backscatter mode." Information about the relative atomic number of the compounds can be obtained in the backscatter mode due to the contrast in brightness between the low atomic number compounds and the compounds with high atomic numbers. For example, iron compounds, which have high mean atomic numbers, tend to be bright white in backscatter mode, while silica compounds, with lower mean atomic numbers, are gray and organic carbon is nearly black. Direct visual inspection of the mulch also provides information on the associations, morphology, and any reaction rims on the particles, all of which provide insight into the geochemical history of the sample. Samples were analyzed on a JEOL 8600 Superprobe located in the Department of Geological Sciences, University of Colorado, Boulder, Colorado.

Samples were received at the University of Colorado Laboratory for Environmental and Geological Sciences between December 2007 and May 2008. The samples arrived frozen under dry ice to minimize potential oxidation of any reduced phases that may have been present. The samples were placed under dry ice until they could be prepared for mounting. The samples were first dried in a sealed chamber using a stream of nitrogen gas. The chamber was equipped with two barbed hose fittings, one to attach to a tank of nitrogen gas and the other to provide an escape route for the moist nitrogen exiting the chamber. The chamber was maintained under a positive nitrogen pressure until the samples were dry. The dried samples were then transferred to a glove box where the process of preparing the epoxy grain mounts was initiated.

A one-gram split of each nitrogen-dried sample was used to prepare epoxy grain mounts within a glovebox with a nitrogen atmosphere. The procedure for preparing the mounts included pouring the sample into a one-inch diameter mold and covering with a thin layer of air-cured epoxy. The grains were then blended with the epoxy using a disposable wood stirring rod and additional epoxy was added. After curing at room temperature within the glove box, the mount was removed and ground flat, forming a cross sectional cut through the grains. Polishing of the mount was performed using successively finer grades of oil-based diamond paste. The grinding and polishing steps involved the use of equipment that was too large to fit in the glove box, so these steps were performed under ambient oxygen conditions. The final step in the preparation of the grain mounts was to apply a thin carbon coating to the surface of the mount or "puck" in order to allow proper conduction during microprobe analysis. The pucks were then stored in the glove box until the electron microprobe analyses could be performed.

2.2.1.2 Carbon

Total organic carbon, total carbon, total inorganic carbon, and moisture content (reported as "drying loss %") analyses were performed by Huffman Laboratories, Inc. in Golden, Colorado.

Moisture content was determined by weighing each as-received sample and then drying the samples in an oven at 105 degrees Celsius (°C) overnight. The dry weight of each sample was then measured and recorded. The moisture content was then calculated by dividing the total weight minus the dry weight by the total weight and multiplying by 100 percent.

Total carbon was determined using high temperature combustion (Method ASTM D5373). Total carbon dioxide was measured by acidifying and heating the sample within a closed system and measuring the liberated carbon dioxide coulometrically (Method ASTM D513). The organic carbon was then determined by subtracting the carbon dioxide carbon from the total carbon.

2.2.1.3 Solid Sample Extractions

The solid sample extractions for analysis of iron- and sulfur- containing minerals were performed by the USEPA NRMRL/GWERD in Ada, Oklahoma and by Microseeps. As the analytical methods used by the USEPA NRMRL/GWERD were unpublished internal standard operating procedures, a brief description of the methods used for each extraction are provided. In cases where the procedures differ only slightly from a published method, the method is cited and only the differences are described. Iron extractions did not provide useful data and are not discussed further.

Sulfur extractions were performed using the methods of Wilkin and Bischoff (2006), and are summarized in **Table 2-6**.

Table 2-6 – Summary of Solid Sample Extraction Methods for Sulfur Minerals

Extraction	Extractants	Target Fe Minerals	Notes
AVS ^a	1M HCl (J.T. Baker)	Amorphous FeS, mackinawite, greigite	
CrRS ^b	1M CrCl ₂ in 0.5M HCl	Elemental S, pyrite	<i>Prepared by passing 1M CrCl₃·6H₂O (Fluka, 98+%) dissolved in 0.5M HCl through a standard Jones reactor</i>

Notes:

a) Acid Volatile Sulfide (mg-S/kg).

b) Chromium-reducible sulfur (mg-S/kg).

2.3 Ground Water Analyses

2.3.1 General Parameters

The general parameters consisted of pH, oxidation-reduction potential, dissolved oxygen, specific conductance, temperature, ferrous iron (Fe⁺²), manganese, sulfide, alkalinity, total organic carbon, and total dissolved solids. The methods used and laboratories that performed the analyses are shown in **Table 2-7**.

Table 2-7 – Summary of Methodology and Laboratories Used for the General Parameters

General Parameter	Method	Laboratory
pH	Direct-reading meter	Measured in the field
Oxidation-Reduction Potential	Direct-reading meter	Measured in the field
Dissolved Oxygen	Direct-reading meter	Measured in the field
Specific Conductance	Direct-reading meter	Measured in the field
Temperature	Direct-reading meter	Measured in the field
Ferrous Iron	Colorimetric, Hach Method 8146	Measured in the field
Manganese	Colorimetric, Hach Method 8034	Measured in the field
Sulfide	Colorimetric, Hach Method 8131	Measured in the field
Alkalinity	Titrimetric, Hach Method 8203	Measured in the field
Total Dissolved Solids	USEPA Method 160.1	USEPA ^a , Microseeps ^b , Test America ^c
Total Organic Carbon	SW-846 Method SW9060	Microseeps

Notes:

- a) Altus AFB and USEPA column study samples.
- b) Dover AFB and Seneca Army Depot Activity samples.
- c) Dugway Proving Ground samples.

The general parameters were collected mainly for use in the PHREEQC geochemical modeling and the results are discussed in that section.

The field measurements were performed with direct-reading meters (*e.g.*, YSI Model 600XL), and a Hach[®] portable colorimeter or titration kit in accordance with manufacturer-specified procedures.

2.3.2 Volatile Organic Compounds (VOCs)

Unfiltered samples for VOC analysis were collected into 40-mL volatile organic analysis (VOA) bottles preserved with HCl, ensuring that no headspace was present. The samples were collected immediately to avoid volatilization losses. VOCs were analyzed by USEPA (Altus AFB), Microseeps (Dover AFB), and Test America (Seneca Army Depot Activity and Dugway Proving Ground) using Method SW-846 Method 8260B.

2.3.3 Methane, Ethene, Ethane, and Acetylene

Methane, ethane, ethane, and acetylene (MEEA) analyses were performed using method AM-20GAX by Microseeps for all sites.

2.3.4 Anions/Cations

Dissolved cations (sodium, potassium, calcium, magnesium, manganese, and iron) and anions (chloride, sulfate, sulfide, phosphate, nitrate, nitrite, and fluoride) were performed by USEPA (Altus AFB) and Microseeps (Seneca Army Depot Activity, Dover AFB, and Dugway Proving Ground), using SW-846 Methods 6010B and 9056A, respectively.

2.3.5 Stable Isotopes

Carbon stable isotope analyses were performed by Microseeps using their internal standard operating procedure.

2.4 Geochemical Equilibrium Modeling

A geochemical model, PHREEQC (Parkhurst and Appelo, 1999), was used to evaluate the saturation state of the reduced iron phases that may be present in the biowalls. PHREEQC is a thermodynamic equilibrium program designed to model chemical speciation in aqueous solutions, determine the saturation states of solutions with minerals and gases, and predict the results of various reactions, such as dissolution of minerals and oxidation.

The modeling shows which reduced iron phases or minerals are saturated (if any) for each solution. Generally, if a solution is at saturation with respect to a mineral, that mineral would be expected to be present within the material in which the water is in contact (e.g., the biowall solids). Minerals which are undersaturated would dissolve when placed in contact with the solution, while minerals that are supersaturated would eventually precipitate the material (assuming the mineral forms at low temperature).

PHREEQC uses a term called the saturation index (SI) to quantify the degree of saturation of a mineral. SI is defined as follows:

$$SI = \text{Log} (IAP/K_{sp})$$

Where IAP is the ion activity product and K_{sp} is the solubility product constant for the phase in question. For phases at saturation, $IAP = K_{sp}$ and $SI = 0$. A negative SI indicates that the phase is undersaturated ($IAP < K_{sp}$) while a positive SI ($IAP > K_{sp}$) indicates the phase is supersaturated. In practice, a range of 0 ± 0.5 SI units is considered saturated due to uncertainties in analytical and thermodynamic data.

2.4.1 Water Analyses Internal Consistency Evaluation

Prior to conducting PHREEQC modeling, the chemical analyses were checked for internal consistency using both charge balance and mass balance relationships. The charge balance was calculated as follows:

$$\frac{(\Sigma(\text{Cations} \times \text{charge}) - \Sigma(\text{Anions} \times \text{charge}))}{(\Sigma(\text{Cations} \times \text{charge}) + \Sigma(\text{Anions} \times \text{charge}))} \times 100 \text{ percent}$$

Where “cations” refers to the molar concentration of positively charged ions in moles per liter (M) and “anions” to the molar concentration of negatively charged ions.

The mass balance was calculated using the following relationship:

$$(\text{TDS}_{\text{Calc}} - \text{TDS}_{\text{Meas}}) / \text{TDS}_{\text{Meas}} \times 100 \text{ percent}$$

TDS is the total dissolved solids and was calculated by summing the concentrations of all species in mg/L. Adjustments were made in cases where the species that would be formed upon evaporation was in a different form than that provided by the laboratory. For instance, silicon reported as “Si” (atomic mass = 28.09 g/mole) was converted to “SiO₂” (atomic mass = 60.09 g/mole) using the factor 2.14 (60.09 g/mole ÷ 28.09 g/mole = 2.14). In addition, the bicarbonate concentration was multiplied by a factor of 0.49 to account for loss of carbon dioxide gas during evaporation.

By evaluating both the mass balance and charge balance, conclusions could be drawn about the accuracy and completeness of the analysis. The possible mass balance and charge balance combinations and the corresponding interpretations are shown in **Table 2-8**.

Table 2-8 – Interpretation of Charge and Mass Balance Results

Mass Balance	Charge Balance	Interpretation ^a
Positive	Positive	Cations are over-reported
Positive	Negative	Anions are over-reported
Negative	Negative	Cations are under-reported and/or one or more important cations were not analyzed
Negative	Positive	Anions are under-reported and/or one or more important anions were not analyzed

Notes:

Note that the interpretation represents the least complex explanation. In some cases, multiple problems with an analysis may have caused the inconsistencies.

A summary of the analyses used for each site and the necessary adjustments to the data based on mass and charge balances is provided in Appendix C.

2.4.2 PHREEQC Thermodynamic Database

The thermodynamic database used by PHREEQC was supplemented to include the iron phases that have been proposed as chlorinated solvent reducing agents as well as other iron phases of interest. The phases that were added and the thermodynamic data used are presented in Appendix C.

2.4.3 Oxidation-Reduction Potential

The oxidation-reduction potential of the solution (also referred to as E_h) is one of the most important parameters for geochemical modeling, but is also one of the most difficult to accurately measure.

E_h was calculated several ways for potential use in the modeling, including the following:

- From electrode measurements collected in the field.
- From the sulfate/sulfide redox couple.
- From the nitrate/nitrite redox couple.

Details on how these E_h values were calculated is included in Appendix C, while additional discussions of the relevance of the different ways of calculating E_h are presented in the results section.

3.0 Results

3.1 Solid Sample Analyses

3.1.1 Electron Microprobe

The electron microprobe was used to identify mineral phases based on their morphology and stoichiometry (from the chemical analyses). The types of iron phases identified were as follows:

- Iron sulfides (iron monosulfides such as mackinawite or troilite and iron disulfides such as pyrite or marcasite) and partially oxidized iron sulfides.
- Iron oxides (magnetite, ferrous oxide, hematite, etc.).
- Hydrated oxyhydroxides (ferrous hydroxide, hydroxyl green rust, etc.).
- Metals (iron).
- Other phases (ilmenite, iron sulfates, sulfate green rust, etc.).
- Ferric oxyhydroxides were rare to absent.

The electron microprobe analyses were fairly definitive for the iron sulfides, because the wavelength dispersive spectrometer on the electron microprobe can analyze for both iron and sulfur, and the phases are not typically hydrated. However, due to the fact the wavelength dispersive spectrometer cannot analyze for hydrogen, determining the difference between hydroxides and hydrated phases was problematic. Theoretically, charge balance relationships could be used to distinguish water from hydroxide. However, when more than one iron oxidation state is possible there are too many degrees of freedom to solve the problem. In such cases, the two possible compositions were reported; however, all concentrations within the range are possible.

An example of such an ambiguous phase was from sample 97S-0088 (Dugway Proving Ground), grain 4 (see Appendix D). In order to determine the mineralogical possibilities for the phase an assumption had to be made as to the oxidation state of the iron. Using the assumption that all of the iron was ferric (Fe^{+3}), the charge balance of the phase was determined (by converting the

mass percentages to molar concentrations). Hydrogen ions or water molecules were then added until charge balance was achieved (if necessary). A similar procedure was employed in which all of the iron was assumed to be ferrous (Fe^{+2}). However, in reality, mixed redox phases are possible. In this report, such a phase is represented by the two end members (100 percent ferric or 100 percent ferrous), realizing that intermediate compositions are possible. Based on the analysis, the two end member phases for grain 4 are, $\text{Fe}_2\text{Ti}_{0.1}\text{O}_{3.5}$ (titanium-bearing hematite) or $\text{FeTi}_{0.1}(\text{OH})_{1.77}$ titanium-bearing ferrous hydroxide, both of which have a composition of 64.2 percent iron, 32.6 percent oxygen, and 3.2 percent titanium. Only the amount of hydrogen (which cannot be quantified on the electron microprobe) varies.

The identification of the sulfide phases was possible in terms of the stoichiometry, but not the actual mineral, which is defined by the crystal structure. For instance iron disulfides could be distinguished from iron monosulfides. However, identifying which iron disulfide (pyrite versus marcasite) or which iron monosulfide (mackinawite versus troilite) generally could not be determined. In addition, identification of sulfides intermediate in composition between iron disulfides and iron monosulfides was also possible. A summary of the common sulfide phases are presented in **Table 3-1**.

Table 3-1 – Iron Sulfide Minerals and the Stoichiometric Compositions

Phase	Formula	Composition	Notes
Pyrite	FeS_2	46.6% Fe, 53.4% S	Precipitation is often kinetically inhibited, usually forms from marcasite.
Marcasite	FeS_2	46.6% Fe, 53.4% S	Intermediate phase in the conversion of pyrrhotite to pyrite. Generally unstable.
Greigite	$\text{Fe}^{+2}\text{Fe}^{+3}_2\text{S}_4$	56.6% Fe, 43.4% S	Does not precipitate directly, generally formed from pyrrhotite, tends to be unstable, converts to marcasite. Contains both ferrous and ferric iron.
Pyrrhotite	Fe_{1-x}S	59.1-63.5% Fe, 36.5-40.9% S	Iron sulfide in which ferrous iron vacancies are charge balanced by ferric iron in the structure.
Troilite	FeS	63.5% Fe, 36.5% S	Pyrrhotite without vacancies. Often referred to as “stoichiometric pyrrhotite”
Mackinawite	FeS_{1-x}	>63.5% Fe, <36.5% S	Thought to be the first phase formed from solution, most iron rich (sulfur poor) phase.

The existence of “amorphous” FeS is in doubt, as a truly amorphous form of iron sulfide has not been identified (Rickard et al., 1995; Wolthers et al., 2003; Rickard, 2006). Even rapidly nucleated forms have been shown to consist of poorly crystalline mackinawite (Morse and Rickard, 2004) and not amorphous FeS. Wolthers et al. (2003) showed that the first phase formed from solution is “nanocrystalline” mackinawite, with crystal diameters of approximately 4 nm. The iron sulfide phases are discussed in more detail in the section on the AVS/CrRS and geochemical modeling results (Sections 3.1.3 and 3.3, respectively).

The following discussions describe the iron sulfides using the descriptive terms: framboidal, granular, crystalline, and coating. For the purposes of this report, the definitions are as follows:

Framboidal – An agglomeration of microcrystals of approximately equal diameter in a spherical form.

Granular – An individual grain of iron sulfide with no visible evidence of agglomeration in the electron microprobe backscatter image (as opposed to a cluster of smaller crystals)

Crystalline – A grain that has an even consistent backscatter image (in terms of tone and brightness) which usually indicates a mineral with an ordered arrangement of atoms.

Coating – A precipitation of a mineral onto the surface of an existing grain.

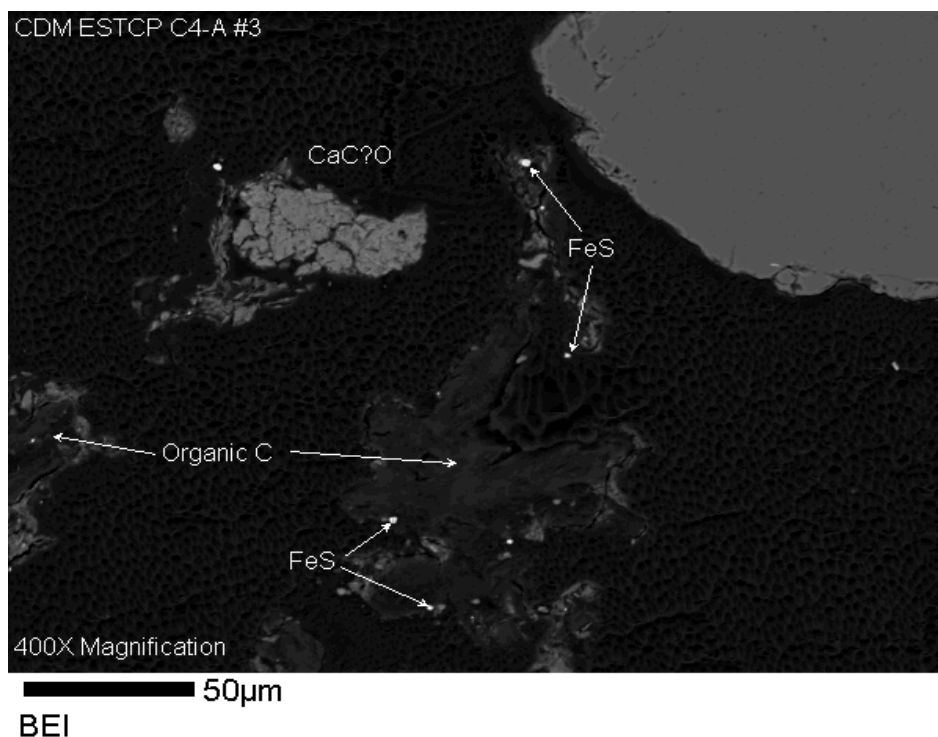
A summary of the phases found in each sample are presented in **Tables 3-2** through **3-6**, while a more detailed evaluation including additional photographs is presented in Appendix D.

3.1.1.1 Altus AFB OU-1 Site

Table 3-2 – Summary of Reduced Iron Phases in Altus AFB OU-1 Samples Analyzed by Electron Microprobe

Sample Identification	Phases and Associations
EPA-C1-A (9.0-10.5 ft)	Granular and framboidal pyrite (FeS ₂) and/or greigite (Fe ₃ S ₄)
EPA-C3-A (5.0-6.5 ft)	Granular iron disulfide (FeS ₂), typically 1 µm diameter in association with organic carbon and clay minerals.
EPA-C4-A (6.5-8 ft)	Granular iron disulfide (FeS ₂), typically 1 µm diameter in association with organic carbon and clay minerals. Also framboidal pyrite and/or greigite.
EPA-C5-A (11.5-13 ft)	Granular iron disulfide (FeS ₂), typically 1 µm diameter in association with organic carbon and clay minerals.
EPA-C6-A (16-17.5 ft)	Granular and framboidal iron disulfide (FeS ₂) and/or greigite, usually associated with organic carbon.
EPA-C7-A (19-20.5 ft)	Granular and framboidal iron disulfide (FeS ₂) and/or greigite and crystalline magnetite (Fe ₃ O ₄)

The iron sulfides present in the Altus AFB OU-1 samples were generally consistent with iron disulfide. The phase was very common, especially as small (one μm) granular particles in association with organic carbon (see **Photomicrograph 1**).

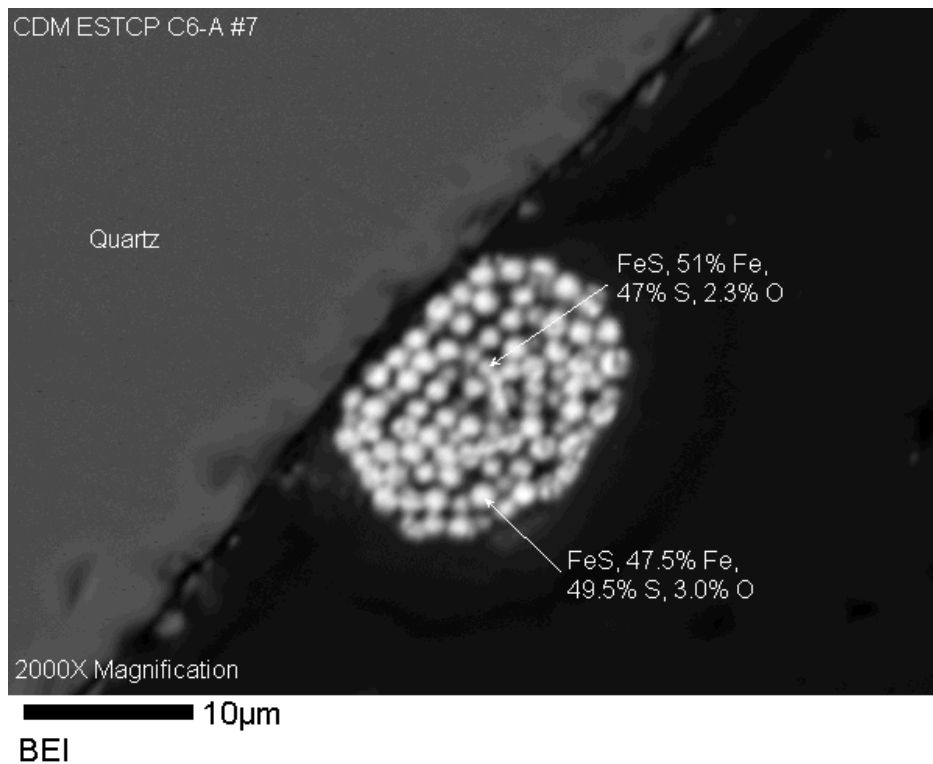


Photomicrograph 1 – Small (~1 μm) Pyrite Grains (White), Associated with Organic Carbon (Black). Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

Of the approximately 151 granular iron sulfide grains identified, 142 were approximately one μm in diameter. Eleven of the iron sulfide grains consisted of larger (6 to 30 μm) framboidal forms, each composed of clusters of hundreds of one- μm to sub-micron size microcrystals. Butler and Rickard (2000) report that framboidal pyrite consists of a close packed array of cubo-octahedral microcrystals, sometimes exhibiting crystallographic orientation of the microcrystals. However, due to the limited magnification of the electron microprobe, the microcrystals appear as blurry dots arranged in a spherical form (see **Photomicrograph 2**). The framboidal forms tended to be liberated (not embedded in organic carbon) and very porous. The framboidal form of pyrite is generally regarded as the most reactive form due to the large specific surface area (Weber et al., 2004).

Analyses were performed on four of the eleven framboidal grains. In general, the framboidal forms were sulfur deficient for an iron disulfide (53.4 percent S), with compositions of 48.7 percent, 50.0 percent, 46.6 percent, and 49.5 percent. These grains could consist of cores of greigite (with 43.4 percent S) or iron monosulfide (36.5 percent S) with iron disulfide rims as proposed by Wei and Osseo-Asare (1995) to account for sulfur deficiencies in pyrite of up to seven percent by weight. The magnetic properties of greigite have been proposed as one possible explanation for the clustering of microcrystals into framboids (Sweeney and Kaplan, 1973;

Morse et al., 1987; Wilkin and Barnes, 1997). However oxygen concentrations ranged from 0.7 to 2.7 percent, so the sulfur deficiency could be due to partial oxidation of the microcrystals (see Appendix D, Attachment 1 for stoichiometries). The small size of the microcrystals made it difficult to focus 100 percent of the electron beam on the particle. Therefore, part of the 1 to 2 μm diameter electron beam often was partially analyzing the epoxy within the grain mount, which would have diluted the analyses and incorporated some of the oxygen in the epoxy into the analysis of the iron sulfide phase.



Photomicrograph 2 – Framboidal Iron Sulfide Grain. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

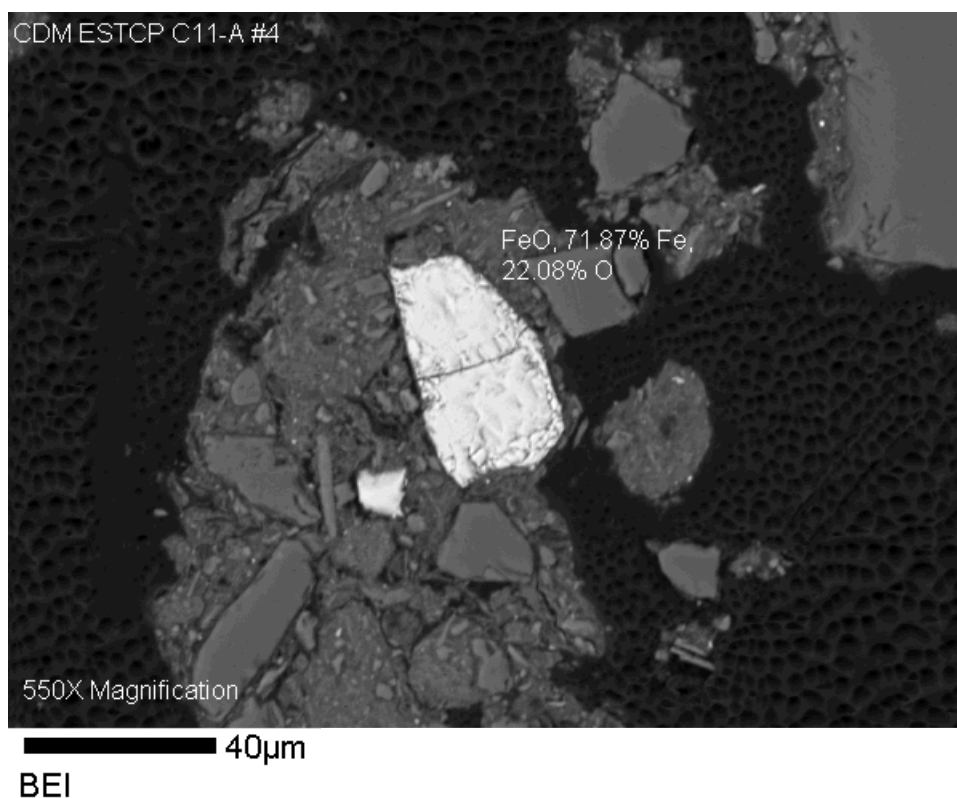
3.1.1.2 Altus AFB SS-17 Site

No iron sulfides or green rusts were identified in the SS-17 site samples. Magnetite (mostly crystalline) was by far the most common form of reduced iron identified in the sample, presumably because magnetite ore was added to the biowall during construction (see **Table 3-3**).

Table 3-3 – Summary of Reduced Iron Phases in Altus AFB SS-17 Samples Analyzed by Electron Microprobe

Sample Identification	Phases and Associations
EPA-C11-A (B04 Transect, 6-7.5 ft)	Crystalline magnetite (Fe_3O_4)
EPA-C13-A (B04 Transect, 12-13.5)	Crystalline magnetite (Fe_3O_4)
EPA-C15-A (B04 Transect, 18-19.5 ft)	Crystalline and secondary ² magnetite (Fe_3O_4) and one grain of iron metal

An example of a typical grain of crystalline magnetite is shown in **Photomicrograph 3**.



Photomicrograph 3 – Crystalline Magnetite. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

² For the purposes of this report, “secondary” refers to a phase that was not an original mineral that has been eroded from a geologic formation (i.e., primary mineral), but was precipitated from solution or was formerly a primary mineral that has been weathered or altered within the aquifer environment to a new composition, structure or morphology.

3.1.1.3 Altus AFB SS-17 USEPA Column Samples

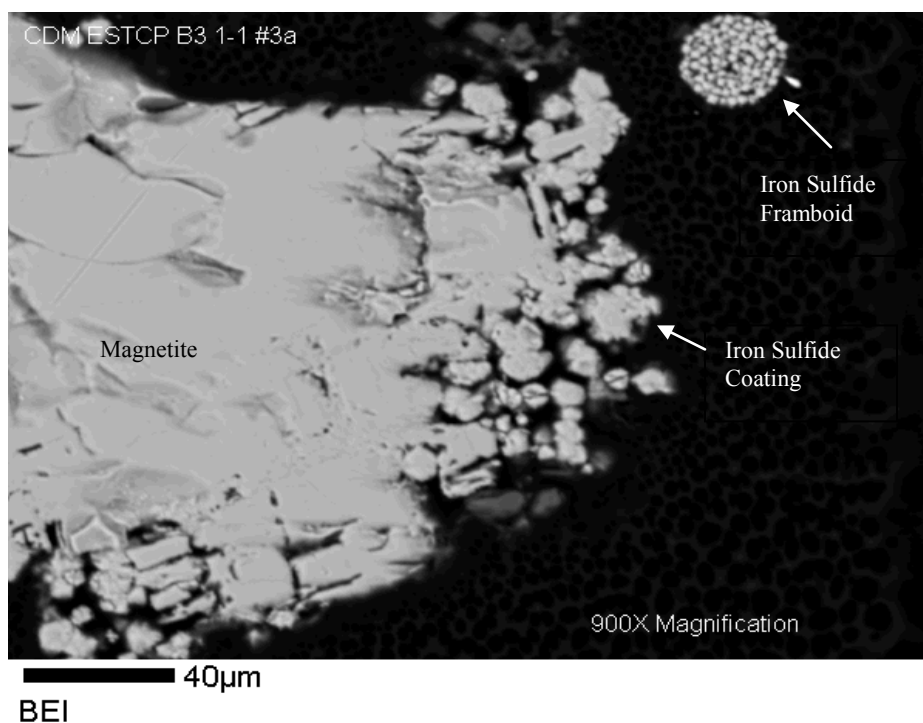
The USEPA column samples had by far the most abundant iron sulfides of any of the sites. Two different forms were identified; framboidal and granular (see **Table 3-4**).

Table 3-4 – Summary of Reduced Iron Phases in USEPA Column Samples Analyzed by Electron Microprobe (EMP)

Sample Identification	Phases and Associations
B3 1-1	Granular Pyrite often coating magnetite (Fe_3O_4). Framboidal iron disulfide or greigite often associated with organic carbon. Spherical silica also noted.
B3 3-1	Iron disulfide associated with magnetite and organic carbon. Partially oxidized iron disulfide and/or green rust.
B3 5-1	Granular iron disulfide often coating magnetite (Fe_3O_4). Framboidal iron disulfide and/or greigite often associated with organic carbon.
B3 7-1	Iron disulfide or greigite associated with magnetite, hematite, and organic carbon. Partially oxidized pyrite and/or green rust (1 grain).

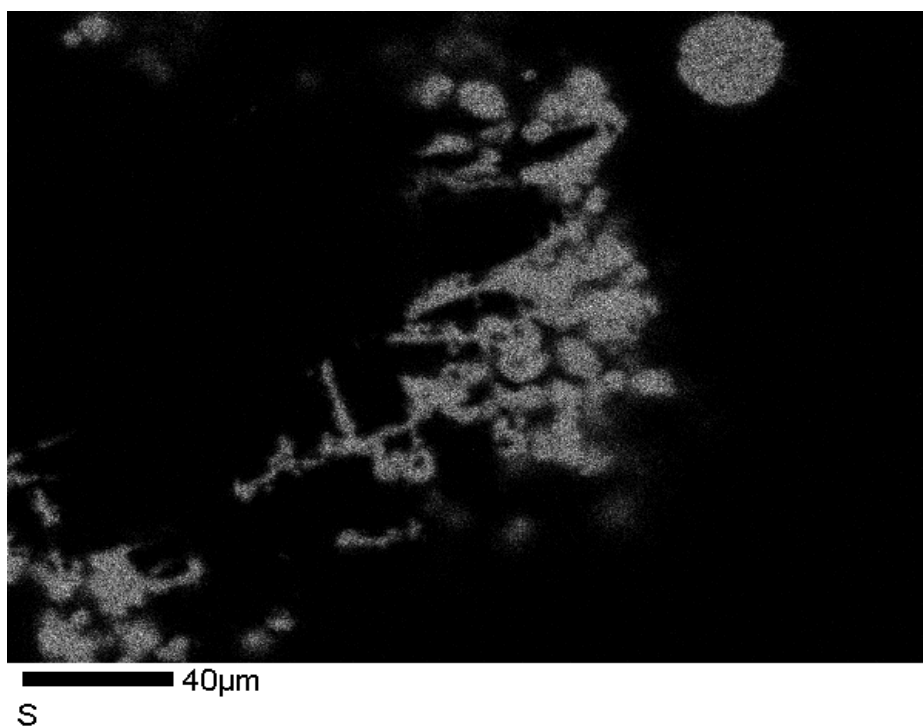
The framboidal form was typically liberated (i.e., not embedded within another larger grain), while the granular form was frequently associated with grains of a crystalline iron oxide consistent with magnetite (Fe_3O_4) and rarely, hematite (Fe_2O_3). Approximately four percent hematite by weight was added to the column sample, while magnetite was likely a component of the river sand used in the mulch formulation. Like the OU-1 samples, some of the iron sulfide phases were slightly sulfur deficient (up to about seven percent) for an iron disulfide, suggesting that the phase could be partially greigite and/or iron monosulfide.

The granular iron disulfide formed coatings on the magnetite and hematite (one grain) as well as filling fractures in the grains. **Photomicrograph 4a** is an image of a composite magnetite/iron disulfide grain. Because iron disulfide and magnetite have similar backscatter intensities, the differences in the phases are difficult to see in **Photomicrograph 4a**. However, **Photomicrograph 4b** shows the same frame with the sulfur distribution represented by white dots, with the greater dot density corresponding to higher sulfur concentrations. The black areas in **Photomicrograph 4b** are the iron oxides, which do not contain sulfur. The close association of the iron oxide and iron sulfide minerals and the coarse nature (i.e., large grain size) of the iron disulfide are evident. Also shown in the photomicrographs is a framboidal iron disulfide (upper right side of frame).



Photomicrograph 4a – Frambiodal Pyrite and Composite Magnetite/Pyrite Grain.

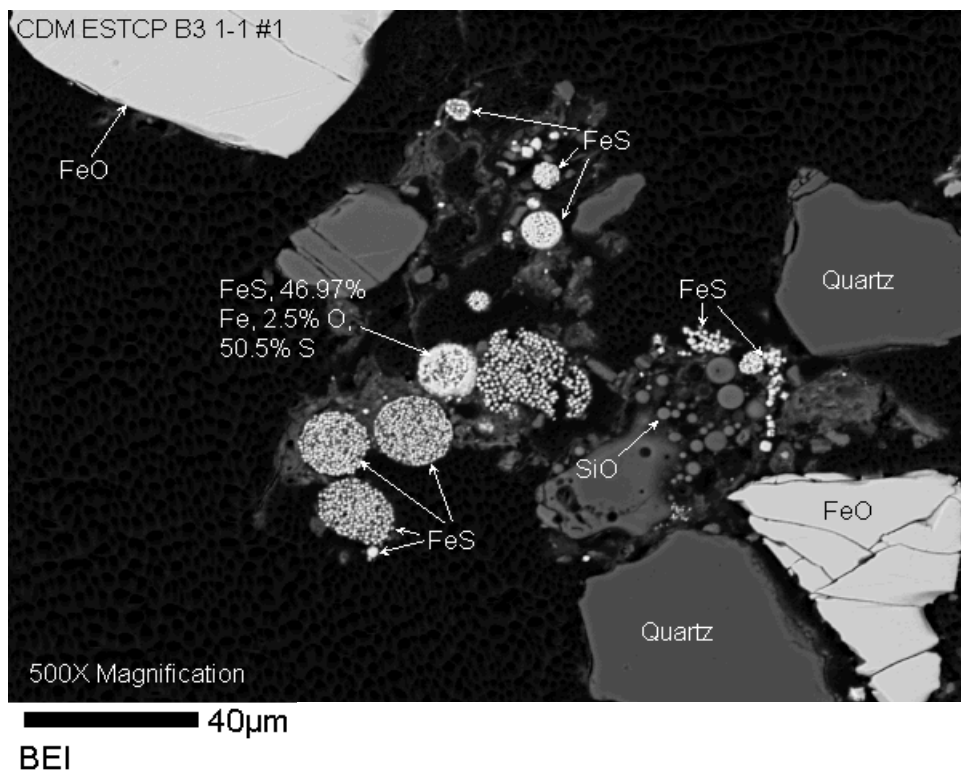
Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.



Photomicrograph 4b – Element Map Showing the Distribution of Sulfur Across the Grain. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

Pyrite coatings appeared to be more common on magnetite grains as opposed to hematite, in which only one coated example was identified. Column sample B3 was amended with four percent hematite by weight, which should have provided abundant surface area for pyrite coatings, but yet coatings on magnetite were much more common. One possible explanation is the differences in the zero point of charge pH (pH_{zpc}) between the two minerals. The pH_{zpc} is the pH at which the electrostatic charge on the mineral is zero. When the solution has a pH less than the pH_{zpc} , then the charge on the mineral is positive, while a pH above the pH_{zpc} results in a negative surface charge. According to Hanoch et al. (2006), iron sulfide coatings begin with adsorption of bisulfide ion (HS^-) onto the surface of the iron oxide. Adsorption of bisulfide is enhanced when the surface charge of the mineral is positive. The pH of the column effluent was 7.35, while the pH_{zpc} for hematite and magnetite are 6.7 and 8.5 (USEPA, 2004), respectively. Therefore, in column B3, magnetite had a positive surface charge and hematite a negative net surface charge, which favored adsorption of bisulfide ion (and subsequent iron sulfide coating) onto magnetite, but not hematite. The rare coating of hematite may be due to the initially lower pH (<6.5) at the beginning of the column study (Shen and Wilson, 2007, Supporting Information).

Photomicrograph 5 shows numerous pyrite framboids, crystalline iron oxides, and a spherical form of silica. The photomicrograph illustrates the abundance of framboidal pyrite within the sample.



Photomicrograph 5 – Framboidal Pyrite, Crystalline Magnetite, Quartz, and Spherical Silica. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

3.1.1.4 Dover AFB

The Dover AFB samples contained a mix of iron monosulfides and iron disulfides, both of which were partially oxidized (Table 3-5).

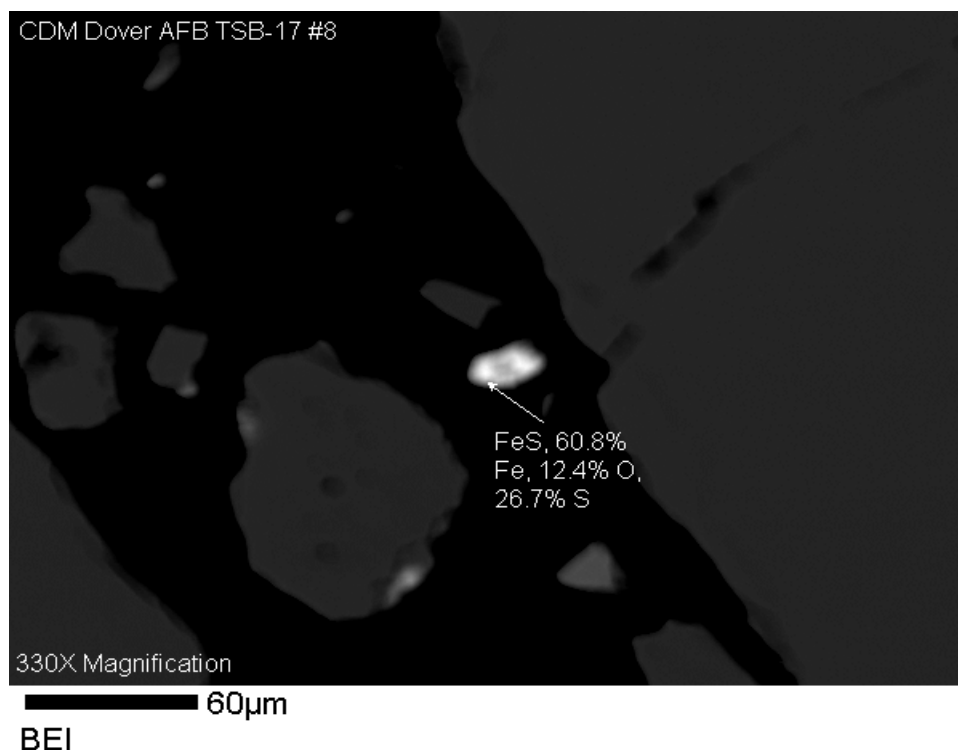
Table 3-5 – Summary of Reduced Iron Phases in the Dover AFB Samples Analyzed by Electron Microprobe (EMP)

Sample Identification	Phases and Associations
DTSB-1-10 (N Transect, UG Wall, 10 ft depth)	Partially to completely oxidized iron disulfide, iron silicate, and possible magnetite and green rust.
DTSB-1-17 (N Transect, UG Wall, 17 ft depth)	Partially oxidized iron sulfides (iron monosulfides and iron disulfides), hydrated ilmenite, ferrous oxide and hydroxide and possible green rust.
DTSB-3-10 (N Transect, DG Wall, 10 ft depth)	Partially oxidized iron sulfides (iron monosulfides and iron disulfides) titanium-bearing ferrous iron oxyhydroxide, and iron silicate.
DTSB-3-16* (N Transect, DG Wall, 16 ft depth)	Partially to completely oxidized iron sulfides (iron monosulfides and iron disulfides). Possible hydrous ferrous hydroxide, ilmenite, iron-silicon sulfate. (also native copper)
DTSB-6-10 (S Transect, UG Wall, 10 ft depth)	Partially to completely oxidized iron sulfides (iron monosulfides and iron disulfides) and ferrous oxysulfate.
DTSB-8-10 (S Transect, DG Wall, 10 ft depth)	Partially to completely oxidized iron sulfides (iron monosulfides and iron disulfides)
DTSB-8-17 (S Transect, DG Wall, 17 ft depth)	Partially to completely oxidized iron monosulfides (3 grains of pseudoframboidal forms) and possible hydroxyl green rust (only 1 grain).
UTSB-16-10* (S Transect, DG Wall, 10 ft depth, dup of DTSB-8-10)	Partially to completely oxidized iron disulfide and hydrous or partially oxidized ilmenite (also native copper)

The particle sizes of the iron sulfides were generally larger than for the OU-1 samples, with a median grain diameter of eight μm and a size range of 2 to 90 μm (statistics, based on 26 grains, are presented in Appendix D). The reason for the larger iron sulfide grain size of the Dover AFB samples compared with Altus AFB OU-1 may be related to a process called “Ostwald Ripening” in which small grains dissolve while larger grains grow (Eberl et al., 1998). The process is driven by the fact that small particles have a higher solubility than larger particles. However, the solubility difference between one- μm crystals and the solubility for 90- μm crystals is negligible, so Ostwald Ripening would typically not be expected to occur. However, in this case, the phase that nucleates from solution (FeS) is different than the phase that is growing within the system (FeS_2). Iron disulfides such as pyrite and marcasite have much lower solubilities than the iron monosulfides, but the nucleation kinetics are slow. Therefore, the first phase to form as the

concentrations of ferrous iron and sulfide increase is mackinawite (an iron monosulfide). The concentrations of mackinawite increase well beyond the solubility limit of pyrite until the saturation state of mackinawite is reached. As discussed elsewhere, iron monosulfides convert to pyrite through various intermediate phases. The grains of pyrite grow simultaneously with the nucleation of mackinawite, as long as ferrous iron and sulfide are continuously added to the system. However, if a change occurs in the system where the concentrations of ferrous iron and sulfide are diluted or the supply is interrupted, then the system may become undersaturated with respect to mackinawite, resulting in dissolution of FeS with simultaneous growth of pyrite. Such a process has been proposed by Morse and Wang (1996) to explain the grain size distribution of authigenic minerals within sediments. The infiltration of oxygenated rainwater or snow melt into the biowalls at Dover would result in a dilution of the biowall porewater, which could initiate the ripening process.

Poorly-formed framboidal pyrites (termed pseudoframboidal) were present, but were rare, with only three examples out of 31 grains (diameters were not recorded for five grains). An example of a typical partially oxidized iron sulfide grain is presented in **Photomicrograph 6**.



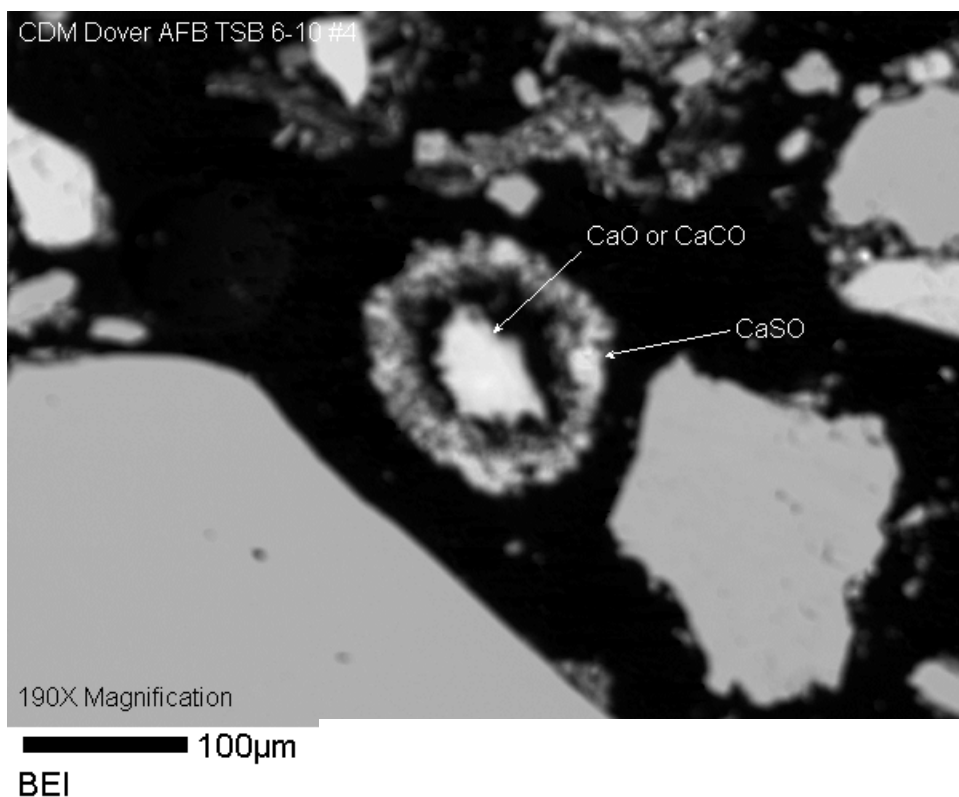
Photomicrograph 6 – Partially Oxidized Granular Iron Sulfide (Original Stoichiometry Obscured by Oxidation).

Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

The sulfides contained a range of oxygen concentrations of 2 to 32 percent, but most were in the 5 to 12 percent range. The iron sulfides in samples from the upgradient wall (TSB1 and TSB6)

had slightly higher median oxygen concentrations (12.1 percent than for the downgradient wall samples (9.0 percent for TSB3 and TSB8). However, there was a substantial variability in the data and the difference may not be significant (see Appendix D, Attachment 1 for the raw data).

Other phases which were present but in lower frequency than the sulfides included possible hydrated ferrous oxyhydroxide, iron silicate, and weathered or partially reacted ilmenite. Secondary coatings of gypsum onto calcite were also noted within a sample from the south transect (where gypsum was added), as shown in **Photomicrograph 7**. The implications of this gypsum/calcite association are discussed in the geochemical modeling section.



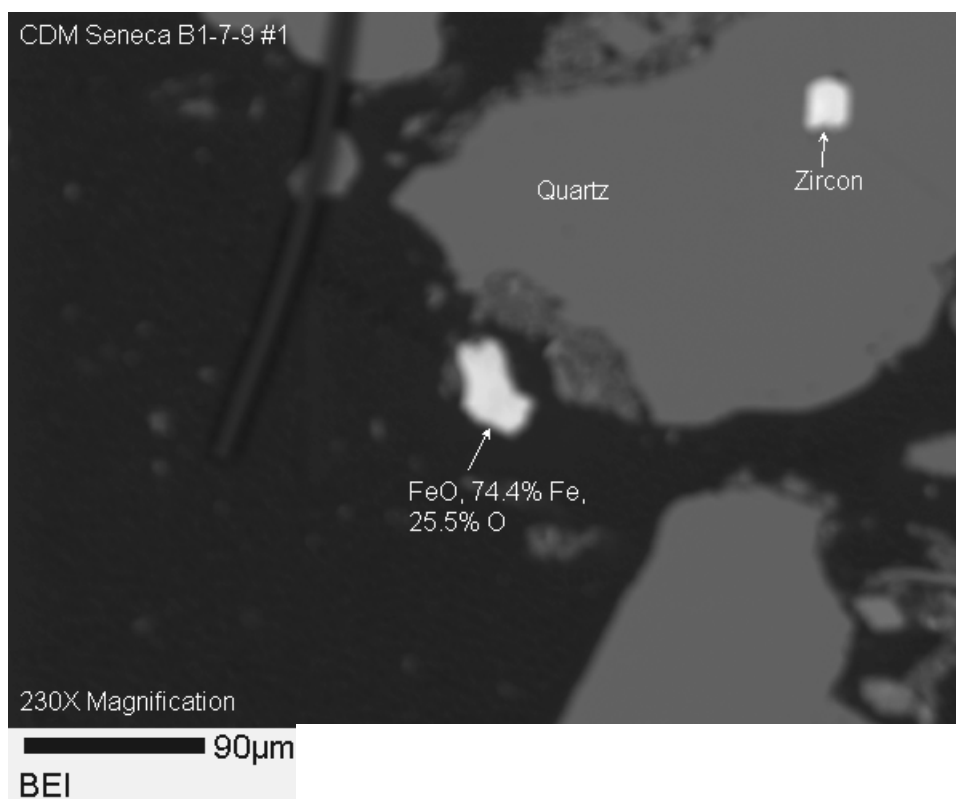
Photomicrograph 7 – Grain of Calcite Coated with Gypsum. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

3.1.1.5 Seneca Army Depot Activity

Sulfide phases were not identified in the Seneca Army Depot Activity samples. The most common forms of reduced iron were magnetite, ilmenite, and possibly ferrous iron oxide (**Table 3-6**). An example magnetite grain is shown in **Photomicrograph 8**.

Table 3-6 – Summary of Reduced Iron Phases in the Seneca Army Depot Activity Samples Analyzed by Electron Microprobe

Sample Identification	Phases and Associations
SA1-9-11 (9-11 ft depth)	Titanium-bearing ferrous oxide.
SA1-6-8 (6-8 ft depth)	Magnetite and/or ferrous oxide.
SB1-7-9 (7-9 ft depth)	Magnetite, ilmenite, and ferrous iron oxide.
SB1-7.5-9.5 (7.5-9.5 ft depth)	Magnetite, iron metal (1 grain), and possible titanium-bearing ferrous hydroxide (1 grain).



Photomicrograph 8 – Iron Oxide Grain Consistent with Magnetite. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

3.1.1.6 Dugway Proving Ground

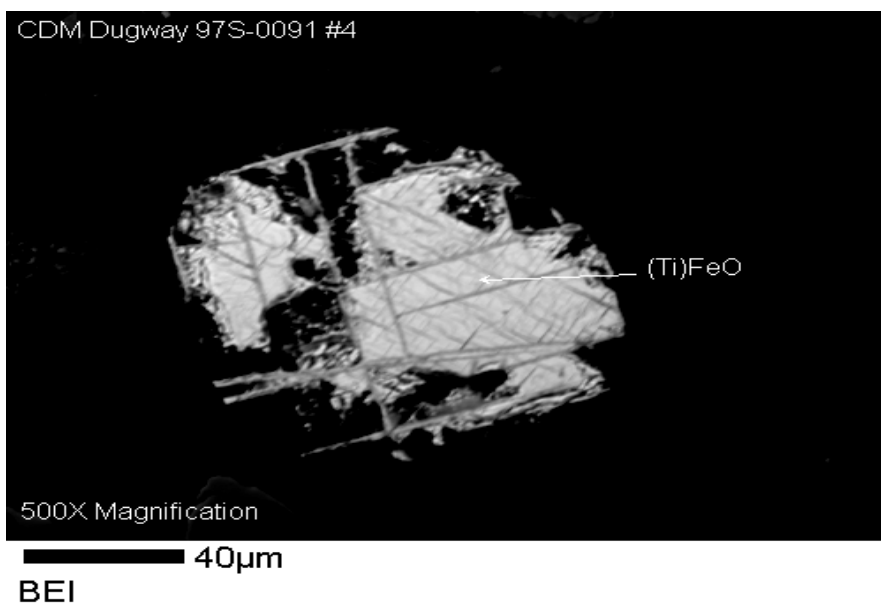
Iron sulfide phases were not identified within the Dugway samples, although a few isolated grains of other metal sulfides (zinc and lead) were found in two of the samples (**Table 3-7**).

Table 3-7 – Summary of Reduced Iron Phases in the Dugway Proving Ground Samples Analyzed by Electron Microprobe

Sample Identification	Phases and Associations
97S-0086	Titanium-bearing hematite and/or titaniferrous hydroxide and partially oxidized zinc sulfide (1 grain)
97S-0087	Titanium-bearing hematite and/or titaniferrous hydroxide and potential hydroxyl green rust (2 grains)
97S-0088	Titanium-bearing hematite and/or titaniferrous hydroxide
97S-0089	Titanium-bearing hematite and/or titaniferrous hydroxide and partially oxidized or hydrated ilmenite.
97S-0090	Titanium-bearing hematite and/or titaniferrous hydroxide and lead-bearing iron oxyhydroxysulfate (1 grain)
97FD-0090	Titanium-bearing hematite and/or titaniferrous hydroxide and partially oxidized lead sulfide (1 grain)
97S-0091	Titanium-bearing hematite and/or titaniferrous hydroxide and magnetite (1 grain)

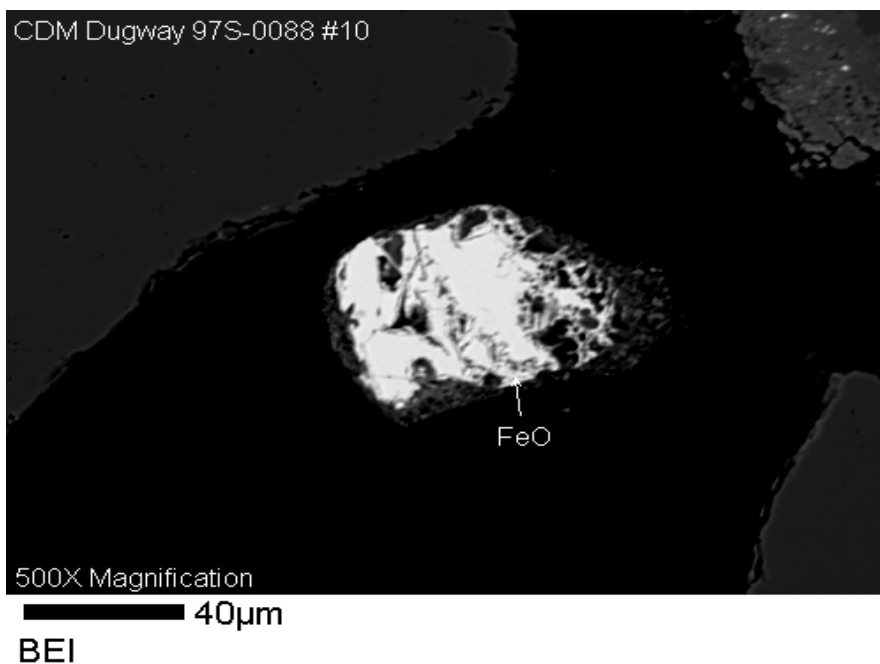
Note that lead and zinc sulfides have a significantly greater backscatter intensity than iron sulfides, which makes them stand out. Therefore, grains of PbS and ZnS are typically easier to find than are iron sulfides. Large areas can be scanned at relatively low magnifications and the bright PbS and ZnS grains can still be found. The vast majority of the sulfur-bearing phases in the samples were sulfate phases (iron hydroxysulfate and barite).

The most abundant form of reduced iron in the phases was in the form of ilmenite (FeTiO_3). The titanium present in the iron oxides is likely due to incorporation of titanium into primary minerals such as magnetite which later weathered to hematite. Some of the grains showed evidence of weathering or reaction, such as deviations from the mineral stoichiometry, and a porous noncrystalline appearance to the grains. Evidence of dissolution of ferric iron minerals such as hematite was common. An example of a grain with a normalized composition of 68.0 percent iron, 30.0 percent oxygen, and 2.0 percent titanium is shown in **Photomicrograph 9**. The composition is consistent with the mineral hematite, as is the near 90° degree parting visible when viewed perpendicular to the c crystallographic axis (the grain just happened to be in the proper orientation). Dissolution of the grain is clearly shown by the cavities and embayments where the mineral has presumably reacted with iron-reducing groundwater.



Photomicrograph 9 – Titanium-Bearing Hematite Showing ~90° Parting. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

Another possibility is that the fractured grain was partially disturbed during grinding or polishing of the sample mount. However, many other examples that cannot be attributed to sample preparation, were identified during the electron microprobe analysis. A grain with a composition consistent with titanium-bearing ferric oxide ($\text{FeTi}_{0.16}\text{O}_{1.8}$) showing a porous character typical of dissolution is shown in **Photomicrograph 10**.



Photomicrograph 10 – Porous and Embayed Titanium-Bearing Ferric Oxide. Chemical formulas in the photomicrograph signify elements that are present and not stoichiometry.

3.1.1.7 Summary of Electron Microprobe Results

A summary of the electron microprobe results for each site is presented in **Table 3-8**. Iron sulfides were identified within the Altus AFB OU-1, USEPA column, and the Dover AFB samples. The OU-1 samples contained framboidal and granular pyrite and/or greigite, but no iron monosulfides were found within the size range which was quantifiable on the electron microprobe ($\geq 1 \mu\text{m}$). The USEPA column samples contained iron disulfide and/or greigite as framboids, $\sim 1 \mu\text{m}$ granular particles, and as $\sim 10 \mu\text{m}$ thick coatings on magnetite. The Dover AFB sulfides consisted of coarse (2 to $90 \mu\text{m}$), partially oxidized (2 to 32 percent oxygen) iron sulfides (iron disulfides, iron monosulfides, and possible greigite).

The Altus AFB SS-17, Seneca, and Dugway samples contained reduced iron phases in the form of hematite, magnetite, and ilmenite, but no iron sulfides within the quantification range of the electron microprobe. The iron oxides were mostly crystalline and often showed signs that partial dissolution had taken place (pitting, embayments, etc.).

Table 3-8 – Summary of Electron Microprobe Results by Site

Site	Major Reduced-Iron Phases and Associations
Altus AFB OU-1	$\sim 1 \mu\text{m}$ granular iron disulfide in association with organic carbon, framboidal iron disulfide and/or greigite, and crystalline magnetite.
Altus AFB SS-17	Crystalline magnetite
Altus AFB SS-17 (USEPA Column)	$\sim 1 \mu\text{m}$ granular iron disulfide in association with organic carbon, framboidal iron disulfide and/or greigite, and crystalline magnetite.
Dover AFB	Partially to completely oxidized iron sulfides (iron monosulfides and iron disulfides). Median grain size $8 \mu\text{m}$.
Seneca Army Depot Activity	Magnetite, ilmenite, and ferrous iron oxide.
Dugway Proving Ground	Titanium-bearing hematite and/or titaniferous hydroxide and partially oxidized or hydrated ilmenite.

3.1.2 Carbon and Moisture

The results of the carbon and moisture content analyses of solid samples are presented in **Tables 3-9 through 3-13**. The majority of the carbon in all samples was organic, reflecting the mulch content. The variability in the data for a given site reflects the heterogeneity of the mulch. The coefficient of variance (CV, $\text{CV} = \text{Standard Deviation}/\text{Mean}$) was high for all of the sites, with a range of 11 to 73 percent for total organic carbon. The high CV is not surprising given the difficulty of thoroughly mixing large volumes of dissimilar materials in the field.

3.1.2.1 Altus AFB OU-1 and SS-17 Sites

The total organic carbon percentages for the OU-1 site are significantly greater than for the SS-17 site.

Table 3-9 - Carbon and Moisture Analysis Results - Altus AFB OU-1 Site

Sample Identification	Moisture Content (%)	Total Carbon (%)	Total Inorganic Carbon (%)	Total Organic Carbon (%)
OU-1 Site				
C1-A	26	4.0	0.48	3.5
C3-A	39	8.6	0.38	8.2
C4-A	41	9.1	0.49	8.6
C5-A	44	12.0	0.51	12
C6-A	42	11	0.44	11
C7-A	39	10	0.43	9.5
Mean	39	9.1	0.46	8.6
Standard Deviation	6.3	2.8	0.05	2.8
Coefficient of Variance (CV) %	16	31	11	33
Median	40	9.5	0.46	9.1

Table 3-10 - Carbon and Moisture Analysis Results - Altus AFB SS-17 Site

Sample Identification	Moisture Content (%)	Total Carbon (%)	Total Inorganic Carbon (%)	Total Organic Carbon (%)
C11-A	24	2.5	0.37	2.1
C13-A	23	3.1	0.28	2.8
C15-A	23	3.4	0.29	3.1
Mean ^b	23	3.0	0.31	2.7
Standard Deviation	0.25	0.47	0.05	0.52
CV %	1.1	16	16	19
Median	23	3.1	0.29	2.8

3.1.2.2 Altus AFB SS-17 USEPA Column Study

The USEPA column samples had slightly more organic carbon than the SS-17 mulch wall. The differences in carbon content are likely due to heterogeneity, as the same materials and fractions of materials were used in both studies.

**Table 3-11 - Carbon and Moisture Analysis Results - USEPA
Column Study (Altus AFB)**

Sample Identification	Moisture Content (%)	Total Carbon (%)	Total Inorganic Carbon (%)	Total Organic Carbon (%)
B3 1-1	31	4.4	0.28	4.2
B3 3-1	33	6.5	0.32	6.2
B3 4-1	34	7.3	0.3	7.0
B3 5-1	28	4.5	0.29	4.2
B3 7-1	33	5.9	0.31	5.6
B3 8-1	27	4.2	0.33	3.9
B3 9-1	28	4.5	0.3	4.2
Mean	31	5.3	0.30	5.0
Standard Deviation	3.0	1.2	0.02	1.2
CV %	10	23	6.7	24
Median	31	4.5	0.30	4.2

3.1.2.3 Dover AFB

The Dover AFB samples had similar amounts of organic carbon as for the USEPA Column samples. The low total inorganic carbon is unexpected, given that limestone was a part of the Dover AFB mulch formulation (**Table 1-1**). The heterogeneity of the mulch and the relatively low number of samples may explain the low total inorganic carbon values measured by the lab.

Table 3-12 - Carbon and Moisture Analysis Results - Dover AFB

Sample Identification	Moisture Content (%)	Total Carbon (%)	Total Inorganic Carbon (%)	Total Organic Carbon (%)
Upgradient Wall				
DTSB-1-10	29	4.8	0.7	4.1
DTSB-1-17	29	5.9	1.2	4.8
DTSB-6-10	28	4.8	1.1	3.7
DTSB-6-17	30	5.3	0.77	4.5
Mean	29	5.2	0.93	4.3
Standard Deviation	0.87	0.52	0.23	0.46
CV %	3.0	10	25	11
Median	29	5.1	0.93	4.3

Table 3-12 - Carbon and Moisture Analysis Results - Dover AFB (cont.)

Sample Identification	Moisture Content (%)	Total Carbon (%)	Total Inorganic Carbon (%)	Total Organic Carbon (%)
Downgradient Wall				
DTSB-3-10	32	6.7	1.2	5.5
DTSB-3-16	31	5.5	0.83	4.6
DTSB-8-10	30	5.6	0.8	4.8
DTSB-8-17	30	5.4	1.0	4.3
UTSB-16-10 (dup)	30	5.0	0.58	4.4
Mean	30	5.6	0.89	4.7
Standard Deviation	1.1	0.65	0.23	0.47
CV %	3.7	12	26	10
Median	30	5.5	0.83	4.6

3.1.2.4 Seneca Army Depot Activity

The Seneca Army Depot Activity samples had a higher total inorganic carbon content than for the other samples, which may reflect the presence of carbonate minerals in the material. The difference in organic carbon between the upgradient wall (A1) and the downgradient wall (B1) may not actually exist, as the sample size was small for each group (N=2).

Table 3-13 - Carbon and Moisture Analysis Results - Seneca Army Depot Activity

Sample Identification	Moisture Content (%)	Total Carbon (%)	Total Inorganic Carbon (%)	Total Organic Carbon (%)
A1 Wall (Upgradient)				
SA1-9-11	31	10	2.6	7.9
SA1-6-8	32	6.5	2.5	4.0
Mean¹	31	8.5	2.5	6.0
Standard Deviation	NA	NA	NA	NA
CV %	NA	NA	NA	NA
Median	31	8.5	2.5	6.0
B1 Wall (downgradient)				
SB1-7-9	30	8.1	3.6	4.5
SB1-7.5-9.5	42	14	2.2	11
Mean^a	36	11	2.9	7.9
Standard Deviation	NA	NA	NA	NA
CV %	NA	NA	NA	NA
Median	36	11	2.9	7.9

Note:

NA - not applicable

3.1.2.5 Dugway Proving Ground

The very low total organic carbon of the Dugway Proving Ground samples likely reflects the fact that solid organic matter in the form of a mulch wall was not used at the site, but rather a liquid organic was injected into the aquifer. The organic carbon percentage for Dugway were about 1/40 those of the other sites. However, the variability in the data is high, with a CV of 73 percent for total organic carbon. The variability suggests that the vegetable oil injection was not evenly distributed throughout the reaction zone. Channeling of the injected vegetable oil along paths of least resistance may explain the variability in the data. Total organic carbon concentrations and possibly TCE removal efficiency may be much higher within the active flow zones. The existing well network may not have intercepted the zones where the majority of the flow and biogeochemical transformation reactions are occurring.

The analysis of total organic carbon does not necessarily indicate how much carbon is available for use as an electron donor, since some forms of organic carbon are more bioavailable than other forms. Lignin is particularly difficult for bacteria to utilize, therefore, organic carbon which has a high percentage of lignin is not as bioavailable as organic carbon with low percentages of lignin.

Table 3-14 – Carbon and Moisture Analysis Results - Dugway Proving Ground

Sample Identification	Moisture Content (%)	Total Carbon (%)	Total Inorganic Carbon (%)	Total Organic Carbon (%)
97S-0086	17	1.0	0.97	0.03
97S-0087	17	1.1	0.99	0.13
97S-0088	19	1.3	1.1	0.12
97S-0089	19	1.0	0.99	0.05
97S-0090	19	1.0	0.95	0.08
97FD-0090	16	1.8	1.5	0.28
97S-0091	20	1.1	0.98	0.07
Mean	18	1.2	1.1	0.11
Standard Deviation	1.5	0.28	0.20	0.08
CV %	8.3	23	18	73
Median	19	1.1	0.99	0.08

3.1.2.6 Summary of Carbon and Moisture Results

A summary of the median carbon and moisture results for each site are presented in **Table 3-15**.

**Table 3-15 – Summary of Median Carbon and Moisture Analysis
Results by Site**

Sample Identification	Moisture Content (%)	Total Carbon (%)	Total Inorganic Carbon (%)	Total Organic Carbon (%)
Altus AFB OU-1	40	9.5	0.46	9.1
Altus AFB SS-17	23	3.1	0.29	2.8
Altus AFB SS-17 USEPA Column	31	4.5	0.30	4.2
Dover AFB UG Wall	29	5.1	0.93	4.3
Dover AFB DG Wall	30	5.5	0.83	4.6
Seneca Army Depot Activity Wall A	31	8.5	2.5	6.0
Seneca Army Depot Activity Wall B	36	11	2.9	7.9
Dugway Proving Ground	19	1.1	0.99	0.08

3.1.3 Solid Sample Extractions

3.1.3.1 Sulfur Extractions

The forms of sulfur, including AVS and CrRS are presented in **Tables 3-16** through **3-22**. The AVS analysis is traditionally considered to be useful for discriminating between iron monosulfides (mackinawite, pyrrhotite, and troilite) and greigite (Fe_3S_4) which dissolve at low pH and the iron disulfides (pyrite and marcasite) which are stable at low pH (Morse et al., 1987; Schoonen and Barnes, 1991; Anderko and Shuler, 1997). There is one iron disulfide that dissolves at low pH called melnikovite, which was isolated from Miocene clays in Russia (cited in Vallentyne, 1963), but this mineral is believed to be relatively rare.

The chromium reducible sulfide (CrRS) test when performed following the AVS test (sequentially) extracts any remaining sulfur in the form of iron disulfide or native sulfur. However, the CrRS test is often done separately on sample splits, in which case all of the sulfur forms are extracted (iron monosulfides, iron disulfides, and native sulfur). By comparing the AVS with the CrRS results, the relative fraction of iron monosulfides to iron disulfides plus native sulfur can be determined.

The AVS and CrRS analyses by Microseeps were performed on separate samples whereas sequential extractions of the same samples were conducted by the USEPA. For comparability, CrRS results provided by Microseeps are presented after subtraction of the AVS results. CrRS results provided by the USEPA are presented as reported.

Altus AFB OU-1 Site

The results for the Altus AFB OU-1 site show that just under half of the iron sulfide sulfur exists as iron monosulfides and the balance as iron disulfides. Because iron disulfides contain twice as much sulfur per mole, the fraction as iron disulfide is even less on a molar basis (using the

median values, 41.4 percent FeS₂ and 58.6 percent FeS on a molar basis). Of the seven OU-1 iron sulfide grains analyzed by electron microprobe none had less than 46 percent sulfur (FeS contains 36.5 percent sulfur) and the grain that contained 46 percent sulfur was diluted by nearly five percent oxygen. The difference between the electron microprobe results (all iron disulfide and/or greigite) and the extraction results can probably be explained by one or more of the following:

- The small number of samples analyzed by electron microprobe and the small sample size (~1 g) combined with the heterogeneity of the iron sulfide distribution
- Dissolution of greigite and/or fine-grained/partially oxidized iron disulfide during the AVS analysis
- Analysis of nanoparticulate iron monosulfides within the pore water or sample during AVS analysis

The small sample size used on the electron microprobe combined with the heterogeneous nature of the iron sulfide distribution could partly explain the differences between the electron microprobe results and the AVS/CrRS extractions. Because the samples had to be maintained under anoxic conditions, drying and homogenization of the samples was not an option. A total of ~6 g of sample from the OU-1 site was analyzed by electron microprobe compared to nearly 16 g (dry basis) used for AVS/CrRS. In addition, the 1.5 to 2 hour spent analyzing each OU-1 sample was not sufficient to scan the entire sample mount. A full “point count” scan generally takes about five hours per sample, not including grain analyses. By contrast, 100 percent of the sample is subjected to the AVS leach. The possibility exists that iron monosulfides were present within the samples, but were not identified. Microchanneling of the groundwater through the mulch (as observed in the USEPA columns) may also have resulted in areas enriched in the more oxidized phases (the microchannels) and areas of unoxidized iron sulfides (in stagnant areas). Under such conditions, one 1-g split of the same core could have different iron sulfide phases than another 1-g split.

The possibility that the framboidal forms consist of the mineral greigite could also explain the differences in the results. Morse and Rickard (2004) state “By far, the most abundant solid components of AVS are believed to be metastable mackinawite and greigite”. The authors also state that under some circumstances pyrite may comprise the dominant AVS solid phase.

As the AVS analysis was performed on wet samples (corrected to a dry basis by determining the moisture content on a subsample), the analysis also captures phases present within the pore water (Morse and Rickard, 2004). Wolthers et al., (2003) found that the first phase to precipitate from solution was a nanocrystalline mackinawite in aqueous suspension. The average diameter of the nanocrystals was four nm. Aller (1977) and DiToro et al., (1990) proposed that nanoparticulate mackinawite was a major component of the AVS within sediments. Given the very large specific surface area of such nanoparticles, the implications to abiotic transformation of chlorinated ethenes could be significant. However, as pointed out by Morse and Rickard (2004), identifying such tiny phases using conventional techniques (such as filtration through a 0.45 µm membrane) is problematic. Rickard (2006) was able to filter nanoparticulate mackinawite by virtue of the high salinity (0.1 molar NaCl) used in his experiments, which resulting in coagulation of the particles to >0.45 µm clumps.

Another possible input to the AVS analysis is sulfide dissolved in the pore water (H_2S and HS^-). Therefore, Morse and Rickard (2004) proposed the following equation to represent the AVS analysis:

$$C_{\text{AVS}} = \Sigma C_{\text{S-2 dissolved}} + \Sigma C_{\text{S-2 minerals}} + \Sigma C_{\text{S-2 nanoparticles}}$$

Where,

C_{AVS} = The total sulfur determined using the AVS method (mg S/kg)

$\Sigma C_{\text{S-2 dissolved}}$ = The dissolved components contributing to AVS (mostly HS^- and H_2S) in mg S/kg

$\Sigma C_{\text{S-2 minerals}}$ = The minerals contributing to AVS (mackinawite, pyrrhotite, greigite, \pm pyrite, \pm marcasite) in mg S/kg

$\Sigma C_{\text{S-2 nanoparticles}}$ = The nanoparticulate component contributing to AVS (mackinawite nanocrystals) in mg S/kg

Table 3-16 – Summary of the Mean AVS and CrRS Analyses – Altus AFB OU1 Site

Sample Identification	AVS mean (FeS) (mg-S/kg)	CrRS mean (mg-S/kg)^a	Interpreted Phase(s)
EPA-C1	490	127	Iron monosulfides
EPA-C3	109	319	Iron disulfides and minor iron monosulfides
EPA-C4	164	294	Iron disulfides and minor iron monosulfides
EPA-C5	366	359	Iron monosulfides and iron disulfides
EPA-C6	233	276	Iron monosulfides and iron disulfides
EPA-C7	219	189	Iron monosulfides and iron disulfides
Median	226	285	Both iron disulfides, and iron monosulfides are important
Mean	263	261	
Standard Deviation	141	87	
CV %	54	54	

Note:

a) Reported CrRS values do not include AVS fraction.

Morse and Rickard (2004) noted similar problems with confirming the presence of iron sulfides detected from an AVS analysis, using electron microscopy, in their case, scanning electron microscopy. They attributed the lack of particulate iron sulfides in the scanning electron microscopy analysis to nanoparticles within the pore water and soil (the magnifications of both the scanning electron microscopy and electron microprobe techniques are not high enough to observe nanoparticles).

Altus AFB SS-17 Site

The results of the SS-17 analyses show that the samples consisted predominantly of iron monosulfides (**Table 3-17**).

Table 3-17 – Summary of the Mean AVS and CrRS Analyses – Altus AFB SS-17 Site

Sample Identification	AVS mean (mg-S/kg)	CrRS mean (mg-S/kg)^a	Interpreted Phase(s)
EPA-C11	351	22	Iron monosulfides and minor iron disulfides
EPA-C13	131	4	Iron monosulfides
EPA-C13A ^b	192	24	Iron monosulfides and minor iron disulfides
EPA-C15	156	45	Iron monosulfides and minor iron disulfides
Median	174	23	Mainly iron monosulfides
Mean	207	24	
Standard Deviation	99	17	
CV %	48	71	

Note:

a) Reported CrRS values do not include AVS fraction.

The fact that no iron sulfide grains were found during the electron microprobe analyses is likely related to the small number of samples (N=3) and the small sample size used. Given a 1.5 to 2 hour analysis time, the effective “detection limit” for finding such phases appears to be about 200 mg/kg. The heterogeneity of the iron sulfides at SS-17 is illustrated by the AVS/CrRS data collected from the BB04 and BB05 transects as part of a previous investigation. The results are summarized in **Table 3-18**.

Table 3-18 – Summary of the AVS/CrRS Analyses Performed at the SS-17 Site as Part of a Previous Investigation^a

Transect	Sample Identification	AVS mean (mg-S/kg)	CrRS mean (mg-S/kg)^a
BB04	bb04w-a	410	699
	bb04w-b	ND	110
BB05	bb05w-a	295	225
	bb05w-b	61	157

Notes:

a) Samples were not collected using the freeze-core technique described in Section 2.

b) Reported CrRS values do not include AVS fraction.

The results indicate that AVS and CrRS results can vary by an order of magnitude within a given transect.

Altus AFB SS-17 USEPA Column Study

The USEPA column samples generally had a mixture of iron disulfides and iron monosulfides, although in some samples one stoichiometry predominated over the other (**Table 3-19**).

Table 3-19 - Summary of AVS and CrRS Results - USEPA Column Study (Altus AFB SS-17 Site)

Sample B3 Slice	AVS mean (mg-S/kg)	CrRS mean (mg-S/kg)^a	Interpreted Phase(s)
1	1,021	2,775	Mostly iron disulfide
2	2,643	105	mostly iron monosulfide
3	2,088	530	mostly iron monosulfide
4	2,158	2,120	Mix of iron monosulfide and iron disulfide
5	1,630	987	Mix of iron monosulfide and iron disulfide
6	1,450	1,518	Mix of iron monosulfide and iron disulfide
7	1,296	1,793	Mix of iron monosulfide and iron disulfide
8	1,190	955	Mix of iron monosulfide and iron disulfide
9	577	1,583	Mostly iron disulfide
Median	1,450	1,518	Both iron monosulfides and iron disulfides are important
Mean	1,561	1,374	
Standard Deviation	641	822	
CV %	41	60	

Note:

a) Reported CrRS values do not include AVS fraction.

Dover AFB

The CrRS analysis for Dover AFB was performed sequentially on the same samples as for AVS. Therefore, the CrRS results represent only the iron disulfide and, if present, native sulfur in the samples (**Table 3-20**). As with the USEPA column samples, the Dover AFB samples had a mixture of iron disulfides and iron monosulfides. In some samples iron monosulfides predominate, while in other iron disulfides predominate, but there is no apparent correlation with the sample depth or which wall the sample was collected from, at least in terms of the iron monosulfide/iron disulfide ratios. However, the total iron sulfide content (as S) is approximately three times higher in the south transect samples compared to the north transect. The addition of gypsum to the mulch mix in the southern section of the biowall is the likely cause of the increased sulfide production in the south transect.

Table 3-20 - Summary of AVS and CrRS Results - Dover AFB

Sample	AVS mean (mg-S/kg)	CrRS mean (mg-S/kg) ^a	Interpreted Phase(s)
North Transect			
TSB1-10	302	176	Mixture of iron monosulfides and iron disulfides
TSB1-17	581	260	Mixture of iron monosulfides and iron disulfides
TSB3-10	821	286	Mixture of iron monosulfides and iron disulfides
TSB3-16	169	114	Mixture of iron monosulfides and iron disulfides
Median	441	218	Both iron monosulfides and iron disulfides are important
Mean	468	209	
Standard Deviation	291	79	
CV %	62	38	
South Transect			
TSB6-10	1,420	1,592	Mixture of iron monosulfides and iron disulfides
TSB6-17	1,539	1,315	Mixture of iron monosulfides and iron disulfides
TSB8-10	1,105	2,114	Mixture of iron monosulfides and iron disulfides
TSB8-17	1,408	1,050	Mixture of iron monosulfides and iron disulfides
Median	1,414	1,453	Both iron monosulfides and iron disulfides are important
Mean	1,368	1,518	
Standard Deviation	185	455	
CV %	14	30	

Note:

a) Reported CrRS values do not include AVS fraction.

Seneca Army Depot Activity

The Seneca Army Depot Activity data show that the total iron sulfides present was an order of magnitude lower than for the previously discussed sites (**Table 3-21**).

Table 3-21 – Summary of AVS and CrRS Results – Seneca Army Depot Activity

Sample	AVS mean (mg-S/kg)	CrRS mean (mg-S/kg)^a	Interpreted Phase(s)
SA1-6-8	63	205	Mostly iron disulfides with minor iron monosulfides
SA1-9-10	65	157	Mostly iron disulfides with minor iron monosulfides
Median	64	181	Iron disulfides are more important
Mean	64	181	
Standard Deviation	NA	NA	
CV%	NA	NA	
SB1-7-9	18	197	Mostly iron disulfides with minor iron monosulfides
SB1-9.5-7.5	23	175	Mostly iron disulfides with minor iron monosulfides
Median	21	186	Iron disulfides are more important
Mean	21	186	
Standard Deviation	NA	NA	
CV %	NA	NA	

Note:

a) Reported CrRS values do not include AVS fraction.

Iron disulfide was the most abundant stoichiometry in all of the Seneca Army Depot Activity samples. Note that no iron sulfide grains at all were identified during the electron microprobe analysis. The very low concentration of iron sulfides, the “nugget effect” and the small sample size used in the electron microprobe analysis (~1 g), and possibly the presence of nanoparticles or other phases in the pore water discussed above may have contributed to the lack of iron sulfides being found during the electron microprobe analysis.

Dugway Proving Ground

Similar to the Seneca Army Depot Activity and SS-17 samples, iron sulfides were detected by AVS/CrRS but not by electron microprobe (**Table 3-22**).

Table 3-22 – Summary of AVS and CrRS Results – Dugway Proving Ground

Sample Identification	AVS mean (mg-S/kg)	CrRS mean (mg-S/kg)^a	Interpreted Phase(s)
097FD-0090	112	43	Mixture of iron monosulfides and iron disulfides
097S-0086	3.2	0.2	Mixture of iron monosulfides and iron disulfides (but overall low in both)
097S-0087	19	68	Mixture of iron monosulfides and iron disulfides
097S-0088	182	112	Mixture of iron monosulfides and iron disulfides
097S-0089	93	0.7	Mostly iron monosulfide
097S-0090	80	28	Mostly iron monosulfide
097S-0091	31	402	Mostly iron disulfide
Median	80	43	Both iron monosulfides and iron disulfides are present
Mean	74	94	
Standard Deviation	62	142	
CV %	84	151	

Note:

a) Reported CrRS values do not include AVS fraction.

Summary of AVS/CrRS Results by Site

The median AVS/CrRS results for each site are summarized in **Table 3-23**.

Table 3-23 - Summary of Median AVS and CrRS Results by Site

Sample Identification	AVS (mg-S/kg)	CrRS (mg-S/kg)^a	Interpreted Phase(s)
Altus AFB OU-1	226	285	Both iron monosulfides and iron disulfides are prevalent
Altus AFB SS-17	174	23	Mainly iron monosulfides
Altus AFB SS-17 USEPA Column	1,450	1,518	Both iron monosulfides and iron disulfides are prevalent
Dover AFB N Transect	441	218	Both iron monosulfides and iron disulfides are prevalent
Dover AFB S Transect	1,414	1,453	Both iron monosulfides and iron disulfides are prevalent
Seneca Army Depot Activity Wall A	64	181	Iron disulfides are more prevalent
Seneca Army Depot Activity Wall B	21	186	Iron disulfides are more prevalent
Dugway Proving Ground	80	43	Both iron monosulfides and iron disulfides are present

Note:

a) Reported CrRS values do not include AVS fraction.

3.1.3.2 Iron Extractions

The iron extractions consisted of ascorbate, dithionite, and 0.5 M HCl leaching solutions. In addition a nitric acid digestion was performed to obtain the total iron content of the sample. Each of the different leach solutions, in theory, should leach a specified form of iron. However, in practice, the selectivity of many extraction methods is poor and the processes and chemical reactions taking place during the extractions are poorly understood (Hlavay et al., 2004). No correlations or trends among the data for the various sites and biogeochemical treatment system performance were observed. Therefore this analysis was not considered to be useful. Extraction and analysis data are included in Appendix A for reference.

3.2 Water Analyses

3.2.1 Volatile Organic Compounds and Methane, Ethene, Ethane, and Acetylene

3.2.1.1 System Effectiveness

In order to correlate the geochemical conditions, design parameters, and solid reduced-iron phases to system performance, a quantitative assessment of the effectiveness of each system must be made. The most basic approach is to look at percent removal of TCE or PCE between the upgradient well and the biowall well. Results of such an analysis are presented in **Tables 3-24** and **3-25** for TCE and PCE, respectively.

Table 3-24 - Summary of TCE Removal Effectiveness by Site

Site	Upgradient Well	TCE Concentration (µg/L)	In-Wall Well	TCE Concentration (µg/L)	Percent Removal
Altus AFB SS-17 West Transect	BB04U	3,930	BB04W	1.45	99.96%
Altus AFB SS-17 East Transect	BB05U	154	BB05W	2.54	98.35%
Altus AFB OU-1	EPA-UMP1	550	MP1	0.105	99.98%
Seneca Army Depot Activity Wall A	MWT-25	26	TEMP-1	3.6	86.2%
Seneca Army Depot Activity Wall B1	MWT-26	2.8	MWT-27	<10	NA ^a
Seneca Army Depot Activity Wall B2	MWT-27	<10	MWT-28	<5	NA ^a
Dugway Proving Ground	TW-25	1,400	TW-28	1,500	-7.1%

Note:

a) Could not be calculated due to one or more non-detect results.

Table 3-25 - Summary of PCE Removal Effectiveness - Dover AFB Site

Site	Upgradient Well	PCE Concentration (µg/L)	In-Wall Well	PCE Concentration (µg/L)	Percent Removal
Dover AFB North Transect - DG Biowall	TS-MW02	5.1	TS-MW03	18	-252.9%
Dover AFB South Transect - DG Biowall	TS-MW07	11	TS-MW08	11	0.00%
Dover AFB North Transect - UG Biowall	TS-MW11	11	TS-MW01	17	-54.6%
Dover AFB South Transect - UG Biowall	TS-MW12	2.4	TS-MW06	2.8	-16.7%

The results indicate that by far the most effective systems are Altus AFB OU-1 and Altus AFB SS-17, followed by Seneca Army Depot Activity. The results for the downgradient wall at Seneca Army Depot Activity (Wall B1/B2), Dover AFB, and Dugway Proving Ground are all negative, because the biowall concentrations were either higher than the upgradient concentration (Dover AFB and Dugway Proving Ground) or the detection limits were too high (Wall B1/B2 at Seneca Army Depot Activity). The negative removals for Dover AFB are likely due to the flat gradient at the site and groundwater flow reversals following precipitation events, as discussed in the historical performance section in the Introduction. The PCE concentrations are generally too low to use in calculations or for drawing conclusions. The Dugway Proving Ground upgradient versus injection zone results only differ by seven percent and probably represent analytical fluctuations on groundwaters which have essentially the same TCE concentrations (i.e., the vegetable oil injection is currently not resulting in any significant TCE removal).

Effectiveness in terms of percent removal requires additional explanation, because some of the systems have much longer residence times and higher TCE concentrations than others. Therefore, overall rate constants were calculated using the following pseudo first-order rate expression (Shen and Wilson, 2007):

$$k_{\text{overall}} = -\ln(C_{\text{DG}}/C_{\text{UG}})/\zeta$$

where,

k_{overall}	=	The overall rate constant for TCE removal from groundwater [1/hr]
C_{DG}	=	The downgradient (biowall) concentration of TCE [µmole/L]
C_{UG}	=	The upgradient concentration of TCE [µmole/L]
ζ	=	The residence time of groundwater within the biowall [hrs]

The results are shown in **Table 3-26** below, while the calculation brief is provided in Appendix E.

Table 3-26 - Overall Rate Constants for the Degradation of TCE

Site	Well Pair	TCE Upgradient C_{UG} ($\mu\text{mole/L}$)	TCE Downgradient C_{DG} ($\mu\text{mole/L}$)	$-\ln(C_{DG}/C_{UG})$	Residence Time ζ (days)	Rate Constant k_{overall} (h^{-1})	TCE Half Life (days)
Altus AFB SS-17	BB04U - BB04W	29.91	0.01	7.90	1.0 to 50	3.29×10^{-1} to 6.59×10^{-3}	0.09 to 4.4
	BB05U - BB05W	1.17	0.02	4.10	1.0 to 50	1.71×10^{-1} to 3.42×10^{-3}	0.17 to 8.4
USEPA Column (Altus AFB SS-17)	Influent-Effluent	19.67	0.13	5.01	17.5	1.19×10^{-2}	2.4
Altus AFB OU-1	EPAUMP-1- MP-1	4.19	0.076	4.01	13.7	2.60×10^{-2}	1.1
Seneca Army Depot Activity	MWT-25 - TEMP-1	0.20	0.027	1.98	16.0	5.15×10^{-3}	5.6
					66.0	1.25×10^{-3}	23

Calculations were not performed for the downgradient biowall at Seneca Army Depot Activity, Dover AFB, and Dugway Proving Ground because the downgradient concentrations were higher than the upgradient concentrations or the detection limits were too high.

The rate constants for Altus AFB OU-1 and the USEPA Column study were the most rapid of all of the sites. The Altus AFB SS-17 field rates have a wide range of rates (3.3×10^{-1} to $6.6 \times 10^{-3} \text{ h}^{-1}$) due to the uncertainty in the residence time within the biowall (1 to 50 days), which can be traced back to a wide range in the calculated groundwater velocity.

As a check on the field-determined rate constants, the literature was searched for abiotic rate constants measured under similar conditions and iron sulfide phases. Most of the literature data were determined from laboratory experiments, because few field data are available. The results, including the experimental conditions, type and quantity of iron sulfide used and the estimated total surface area are presented in **Table 3-27**.

Table 3-27 – Summary of TCE Degradation Rates by Iron Sulfides and Reaction Products from the Literature

Study	Form of Iron Sulfide	Specific Surface Area of Iron Sulfide (m ² /g)	Total Iron Sulfide Surface Area (m ² /L solution) ^a	pH	Reaction Products	Rate Constant (h ⁻¹)
Butler and Hayes, 2001	Freshly prepared poorly crystalline mackinawite	0.05	0.5	7.3	acetylene (76%) <i>cis</i> -DCE (11%) TCE remaining (12%)	5.0 x 10 ⁻⁴
				8.3	acetylene (65%) <i>cis</i> -DCE (6%) VC (<1%) TCE remaining (9%)	1.5 x 10 ⁻³
				9.3	acetylene (96%) <i>cis</i> -DCE (2%) TCE remaining (6%)	2.0 x 10 ⁻³
Butler and Hayes, 1999	Freshly prepared poorly crystalline mackinawite	0.05	0.5	8.3	acetylene (71%) <i>cis</i> -DCE (7%) VC (<1%)	1.37 x 10 ⁻³ (TCE→acetylene) 1.17 x 10 ⁻⁴ (TCE → <i>cis</i> -DCE)
Sivavec et al., 1995	Troilite		0.5	Not given	acetylene (75%) <i>cis</i> -DCE, VC, ethene, ethane, and other C2-C6 carbon (15-20%)	1.15 x 10 ⁻³
Jeong and Hayes, 2007	Freshly prepared poorly crystalline mackinawite nanoparticles	284	2,840	8.3	acetylene (76%) <i>cis</i> -DCE (4%) TCE remaining (17%)	2.12 x 10 ⁻³

Table 3-27 – Summary of TCE Degradation Rates by Iron Sulfides and Reaction Products from the Literature (cont.)

Study	Form of Iron Sulfide	Specific Surface Area of Iron Sulfide (m ² /g)	Total Iron Sulfide Surface Area (m ² /L solution) ^a	pH	Reaction Products	Rate Constant (h ⁻¹)
Weerasoriya and Dharmasena, 2001	4 µm particles of crystalline pyrite	1	2	6.5	acetylene (NQ) 1,1-DCE (NQ), <i>cis</i> -DCE (4-5%) TCE remaining (20%)	1.45 x 10 ⁻²
Lee and Batchelor, 2002	Ground crystalline pyrite (63 - 250 µm diameter)	27.8	2,335	8.3	acetylene (43%) <i>cis</i> -DCE (3%) ethene (2%) TCE remaining (50%)	6.63 x 10 ⁻²
Shen and Wilson, 2007	Iron sulfides generated using SS-17 mulch mix and site groundwater within a series of columns	Not reported	Not reported	6.3 to 7.5	carbon dioxide (11-53%) <i>cis</i> -DCE (<1%), ethanol ^b and acetate ^b	8.33 x 10 ⁻³ to 2.29 x 10 ⁻²

Notes:

a) Calculated by multiplying the specific surface area in m²/g by the concentration of iron sulfide added in g/L.

b) Assumed to have been produced via fermentation, but not measured.

NQ – Not quantified.

The VOC removal rates at the Altus AFB OU-1 and SS-17 sites were generally greater than the abiotic rates calculated for many of the laboratory studies, which were conducted under controlled conditions. The main differences between the laboratory studies and the field results were; 1) in the field systems fresh iron sulfide was continually being produced, whereas in the laboratory studies a finite quantity of iron sulfide was added at the beginning of the experiment, 2) the field systems contain organic carbon, which probably results in biological reactions that do not occur in the laboratory studies. The surface area of the iron sulfide, and the degree of crystallinity and the identity of the mineral phase all factor into the abiotic rate. In addition, the presence of mulch in the field systems results in sorption of VOCs in the biowalls. Sorption of VOCs may have affected overall removal rates either by retarding VOC transport or by directly affecting reaction rates via a concentration effect.

The rates provided for the field sites represent the overall rate of TCE transformation from both biological and abiotic processes, while the laboratory studies are mainly abiotic rates (no substrate was provided and in some cases a biocide was used). Therefore, to obtain a better

understanding of the rates and to break out the relative contribution of the abiotic process, the abiotic versus biological transformation processes were evaluated for each of the field sites.

3.2.1.2 Biological vs Abiotic Transformations

The VOCs evaluated included PCE (for Dover AFB only), TCE, *cis*-1,2-DCE, and VC. The concentration of each parameter were plotted against distance to determine if the VOC concentrations represent a “divergent” or “parallel decrease” trend as defined by Brown et al., (2007). A divergent trend is characterized by the loss of the parent VOC (such as TCE or PCE) with the simultaneous production of daughter products (such as *cis*-1,2-DCE and VC). A divergent pattern is characteristic of biotic dechlorination. A parallel decrease is in when the chlorinated solvents all decrease concurrently (without accumulation of daughter products), which is characteristic of abiotic transformation. The trend plots for each site are included as **Figures 3-1** through 3-6 Acetylene was analyzed but was not included on the charts because a small number of the analyses were above the analytical detection limit.

Altus AFB OU-1 Site

The Altus OU-1 site has a divergent VOC trend, with TCE and *cis*-1,2-DCE decreasing and VC increasing within and down-gradient of the biowall (**Figure 3-1**).

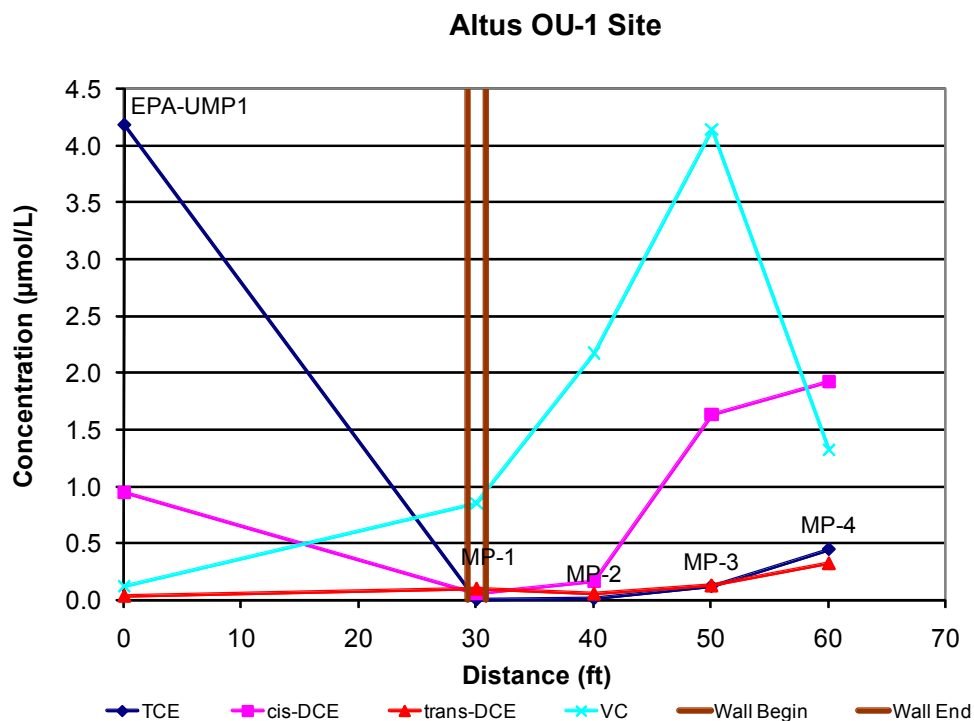


Figure 3-1 - Concentration vs Distance Plot for the Altus AFB OU-1 Site

The trend suggests that the transformation is, at least in part, biological. The buildup of VC may be due to the fact that the abiotic transformation rate for *cis*-1,2-DCE conversion to acetylene by pyrite is 1.6 times slower than for TCE transformation to acetylene (Lee and Batchelor, 2002a). The *cis*-1,2-DCE concentration in the upgradient well was 0.95 μM and the VC concentration was 0.12 μM . In the in-wall sample, *cis*-1,2-DCE was 0.05 μM and VC was 0.85 μM . Therefore, 0.78 μM of *cis*-1,2-DCE was converted to VC ($0.85 \mu\text{M VC DG} - 0.12 \mu\text{M initially present UG} = 0.78 \mu\text{M}$), presumably by biotical reductive dechlorination. The fraction of the *cis*-1,2-DCE converted to VC was 82 percent ($0.78/0.95 \times 100 \text{ percent} = 82 \text{ percent}$), the remaining *cis*-1,2-DCE was either converted to acetylene by abiotic processes, or some of the VC was originally created biotically was further degraded by biotic (to ethene) or abiotic (to acetylene) processes. Ethene, ethane and acetylene were all below the analytical detection limits, indicating that biotic transformation of VC may have been limited, and any acetylene produced via abiotic transformation was quickly transformed by fermenters into organic acids and alcohols.

Altus AFB SS-17 Site

The Altus AFB SS-17 transects B4 and B5 both show a similar trend in chlorinated solvent concentrations. The initial concentrations of TCE and *cis*-1,2-DCE decrease to below the detection limit within the biowall without the simultaneous buildup of daughter products, which is indicative of abiotic transformation.

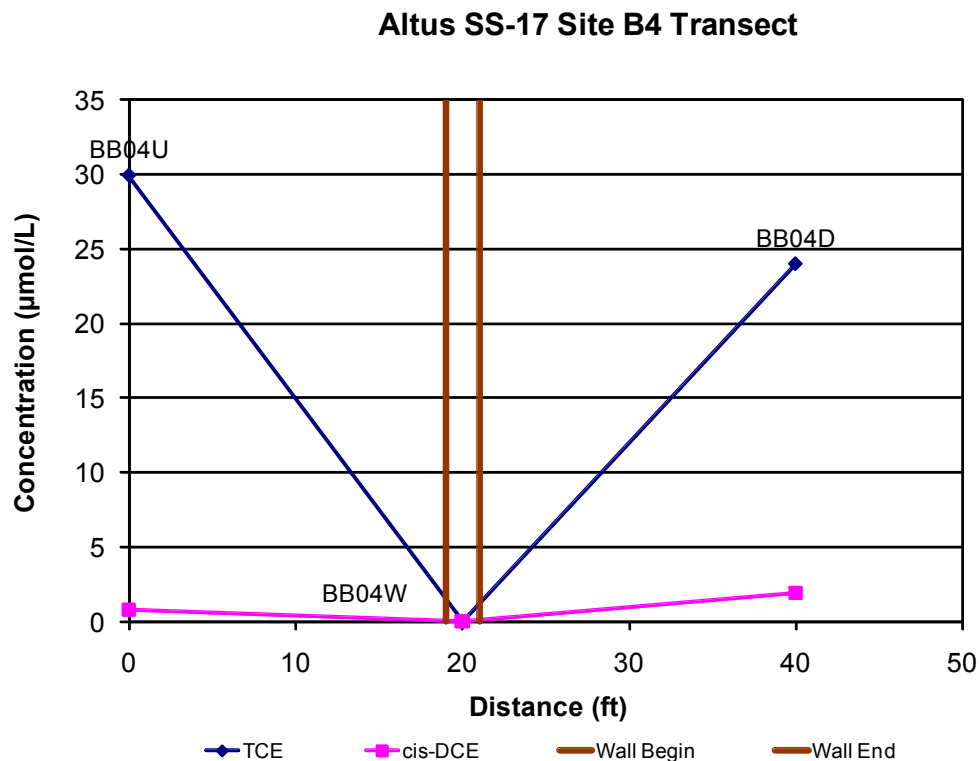


Figure 3-2 - Concentration vs Distance Plot for the Altus AFB SS-17 Site B4 Transect

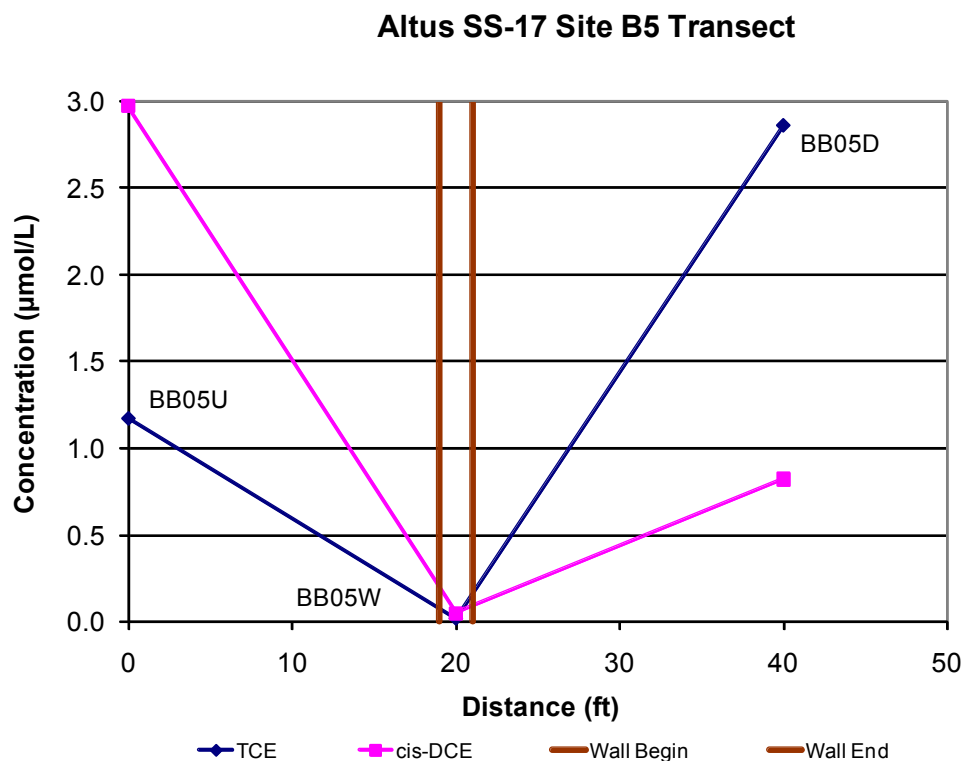


Figure 3-3 - Concentration vs Distance Plot for the Altus AFB SS-17 Site B5 Transect

The increase of VOCs downgradient is likely due to leakage of groundwater around and/or under the biowall. Concentrations of ethene, ethane, and acetylene were all below the analytical detection limits for all samples.

Minor amounts of 1,1-DCE were detected in downgradient samples BB04D and BB05D, but not within the wall. 1,1-DCE is one of the possible transformation products of TCE abiotic degradation by pyrite (Weerasooriya and Dharmasena, 2001).

Dover AFB

The Dover AFB North Transect, exhibits a buildup of *cis*-1,2-DCE and to some extent TCE in the upgradient wall (as has been the case historically for this transect). However, PCE also increases slightly, which is likely due to decreasing PCE concentrations in the upgradient well over time, which would cause PCE to desorb from the biowall materials (**Figure 3-4**).

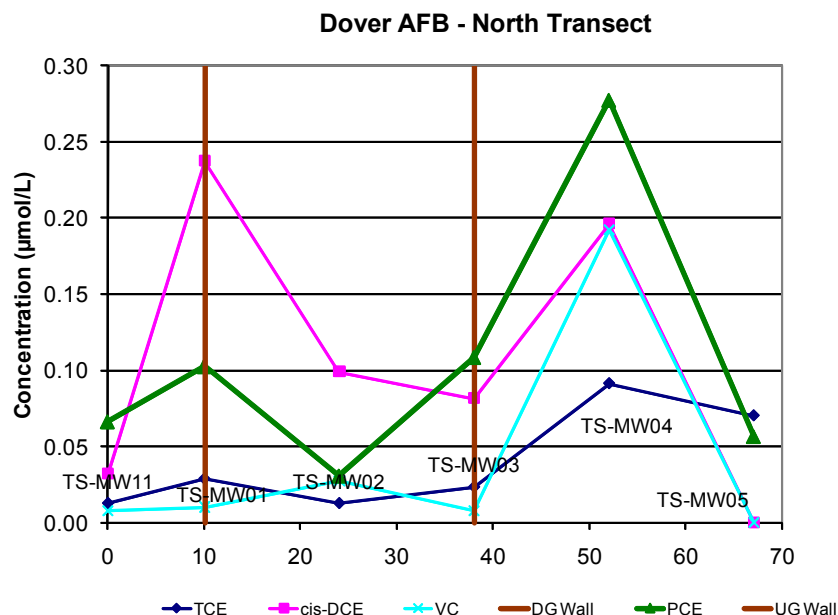


Figure 3-4 – Concentration vs Distance Plot for the Dover AFB Site, North Transect

The downgradient wall appears to have less of a biological component, as daughter products such as *cis*-1,2-DCE and TCE do not appear to be building up. Possible reversals in the groundwater flow direction appear to have obscured the trends, for example the increase in PCE concentrations from the between walls well (TS-MW02) to the downgradient wall well (TS-MW03).

Significant biological transformation is taking place within the aquifer downgradient of the second wall and/or significant leakage under or around the walls is taking place.

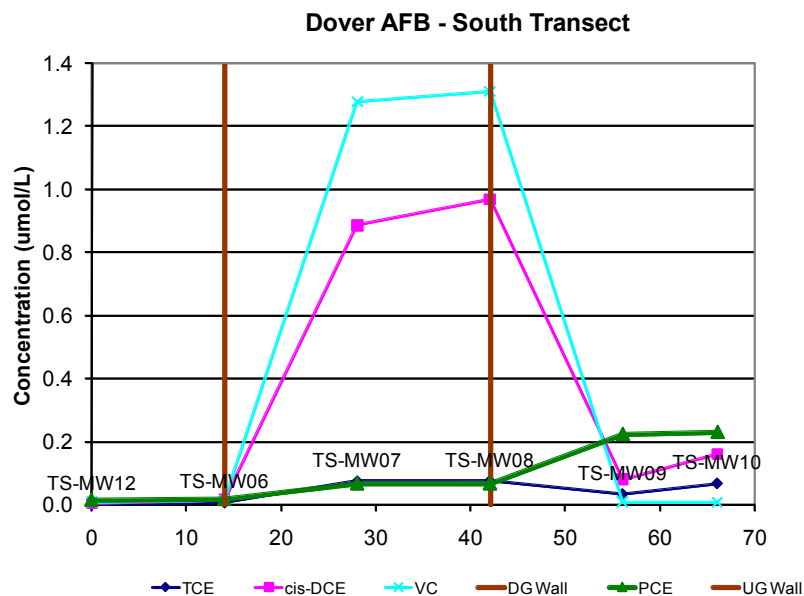


Figure 3-5 – Concentration vs Distance Plot for the Dover AFB Site, South Transect

The South Transect does not exhibit the biological buildup of daughter products in the first wall, however, the VOC concentrations in the upgradient well were very low to start with (**Figure 3-5**). Very little transformation appears to be taking place in the downgradient wall, although the trends could be obscured by groundwater flow reversals.

Downgradient of the second wall, the VOC trend is largely parallel, with all parameters except PCE decreasing concurrently, suggesting that abiotic transformation is occurring downgradient.

Methane concentrations within the south transect walls (gypsum added) was about a third of those measured for the north transect (no gypsum added). The added sulfate in the south may have provided the sulfate-reducing bacteria with a better ability to compete with the methanogens for the available substrate.

Seneca Army Depot Activity

The plume trend diagram for the Seneca Army Depot Activity site is presented in **Figure 3-6**.

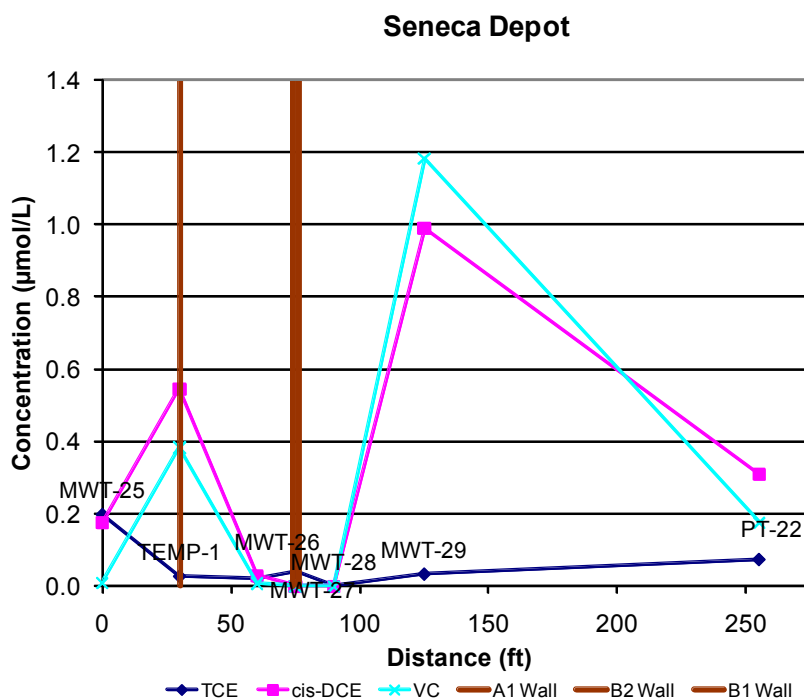


Figure 3-6 – Concentration vs Distance Plot for the Seneca Army Depot Activity

The decrease in TCE that occurs within biowall A is accompanied by an increase in *cis*-1,2-DCE and VC, but not an increase in ethane or ethene. Within Walls B1 and B2, none of the evaluated VOCs were above the detection limit. However, in the well upgradient of biowall B (MWT-26) VOC concentrations were low (2.8 µg/L for both parameters). Downgradient of biowall B, ethene concentrations increased dramatically to 200 µg/L (November 2007 data) suggesting biotransformation of VC has taken place.

Dugway Proving Ground

The TCE results for the upgradient well were higher than for the injection well for Dugway, so a plot was not constructed. In addition, all of the historical VOC data indicate that there is an insignificant change in concentrations from the upgradient well to the injection zone well to the downgradient wells, suggesting that neither biotic nor abiotic transformation is taking place.

Comparison of Sites

For the purposes of this investigation, the degree of abiotic degradation (vs. biological degradation) was quantified using the following VOC mass balance equation:

$$f_{\text{abiotic}} = (\Sigma \text{VOC}_{\text{UG}} - \Sigma \text{VOC}_{\text{biowall}}) / \Sigma \text{VOC}_{\text{UG}}$$

where,

f_{abiotic}	=	the fraction of VOC loss attributable to abiotic transformation [$\mu\text{mol}/\mu\text{mol}$]
$\Sigma \text{VOC}_{\text{UG}}$	=	the sum of the VOCs (TCE + <i>cis</i> -1,2-DCE + VC + ethene + ethane) at the upgradient location (μM)
$\Sigma \text{VOC}_{\text{biowall}}$	=	the sum of the VOCs at the downgradient (biowall) location (μM)

The following assumptions were made:

- All abiotic transformation reactions result in complete mineralization (conversion to CO₂ and H₂O) or to a compound that is not part of the biological reductive dehalogenation reaction pathway (TCE → *cis*-DCE → VC, etc.).
- The VOC concentrations at the upgradient location are the same as at the upgradient edge of the biowall (just before entering the biowall). In other words, no attenuation, dilution, or degradation occurs within the aquifer between the upgradient location and the biowall.
- Reductive biological transformation of TCE does not proceed beyond ethene or ethane.
- Adsorption of VOCs onto the mulch can be considered negligible once the adsorption sites become saturated.

The first assumption, that all of the products are converted to carbon dioxide is supported by the ¹³C results of the USEPA column study (Shen and Wilson, 2007). The production of VOCs such as *cis*-1,2-DCE and biological reductive dechlorination reaction products do occur, as illustrated by the literature studies (**Table 3-35**), however, they generally represent a small fraction of the abiotic reaction products. Butler and Hayes (1999) found that the chloroelimination reaction that produces acetylene was an order of magnitude faster than the abiotic reaction that produces *cis*-1,2-DCE, which may explain the dominance of acetylene production.

While the literature studies almost all agree that acetylene (C₂H₂) is the major product of the abiotic chloroelimination reactions occurring in their systems, they do not explain why acetylene accumulates as the TCE transformation proceeds rather than degrading. The reason for the buildup of acetylene in the laboratory batch studies, but not in the USEPA column study or field systems is thought to be due to the transformation of acetylene to ethanol and acetate via

fermentation, which are in turn oxidized to carbon dioxide by sulfate-reducing bacteria (Shen and Wilson, 2007) and/or methanogenic bacteria (Buccambusco et al., 2007a). Such fermentation reactions are unlikely to occur in the laboratory systems which did not contain organic carbon substrate.

The assumption that the VOC concentrations in the upgradient well are equivalent to those of the groundwater entering the biowall is generally fairly good, as the upgradient wells are fairly close to the biowalls (10 to 20 feet).

The degradation of biologically-produced ethane via oxidation to carbon dioxide is possible, which would cause the fraction of the TCE transformation due to abiotic reactions to be slightly over-predicted.

Adsorption of TCE onto the mulch is likely to be significant during the first several months of operation of the biowall. Calculations show (Appendix E) that for site SS-17, transect BB04 about 80 percent of the TCE is removed from the first pore volume of groundwater to pass through the biowall (using a K_{oc} of 21 L/kg, an f_{oc} of 0.0281, a total porosity of 0.25, and a soil bulk density of 1.65 g/cm³). However, after about 20 pore volumes (see Appendix E), the adsorption sites on the organic carbon become saturated, at which point the organic carbon TCE concentration is in equilibrium with the groundwater concentration at that point within the biowall (the equilibrium will continually shift at increasing distance into the biowall as the aqueous TCE concentrations are decreased by transformation reactions).

The results of the calculations are presented in **Table 3-28**.

Table 3-28 - Summary of the Abiotic Contribution to the Transformation of PCE or TCE

Site	Well Pair (UG-Biowall)	UG Total VOCs (μmol/L)	Total DG VOCs (μmol/L)	% Abiotic	Notes
Altus AFB SS-17 West Transect	B04U-BB04W	30.76	0.0457	99.85%	
Altus AFB SS-17 East Transect	B05U-BB05W	4.16	0.0897	97.84%	
Altus AFB OU-1	EPA-UMP1 - MP1	5.26	0.91	82.70%	
USEPA Column	Influent-Effluent	19.6	0.29	98.50%	Shen and Wilson (2007) calculated 49% to 88% abiotic
Dover AFB North Transect - DG Biowall	TS-MW02-TS-MW03	0.170	0.222	-36.7%	Total VOCs increase from UG to DG wells
Dover AFB South Transect - DG Biowall	TS-MW07 - TS-MW08	2.31	2.42	-6.9%	Total VOCs increase from UG to DG wells
Dover AFB North Transect - UG Biowall	TS-MW11 - TS-MW01	0.119	0.379	-204%	Total VOCs increase from UG to DG wells
Dover AFB South Transect - UG Biowall	TS-MW12 - TS-MW06	0.030	0.0545	-91.5%	Total VOCs increase from UG to DG wells
Seneca Army Depot Activity Wall A	MWT-25 - TEMP-1	0.38	0.96	-153%	Total VOCs increase from UG to DG wells

Table 3-28 - Summary of the Abiotic Contribution to the Transformation of PCE or TCE (cont.)

Site	Well Pair (UG-Biowall)	UG Total VOCs (μmol/L)	Total DG VOCs (μmol/L)	% Abiotic	Notes
Seneca Army Depot Activity Wall B1	MWT-26 - MWT-27	0.058	0.038	35%	
Seneca Army Depot Activity Wall B2	MWT-27 - MWT-28	0.039	<0.0005	>98.69%	
Dugway Proving Ground	TW-25 - TW-28	10.7	11.42	-7.14%	Total VOCs increase from UG to DG wells

Abiotic transformation appears to be the dominant process where significant VOC degradation is occurring, especially for the Altus AFB sites. A relationship between the sites with the fastest overall rate and the highest percentage of abiotic transformation generally holds true. The exception is the Seneca Army Depot Activity Biowall A, which had a significant overall degradation rate of TCE (TCE concentrations decreased) but the overall VOC concentrations increased. Apparently, some degree of desorption was occurring simultaneously with degradation, perhaps in response to a decrease in the upgradient VOC concentrations. Seneca Army Depot Activity Biowalls B1 and B2 had increasing TCE concentrations (so the TCE rate could not be calculated), but the overall concentration of VOCs decreased. Because TCE was not created from degradation of PCE, again, desorption was likely occurring concurrently with abiotic and biotic degradation.

The higher abiotic prediction for the USEPA column sample (98.5 percent abiotic) compared to the range obtained by Shen and Wilson (2007) of 50 to 88 percent is likely related to one of the assumptions made by the authors in order to calculate the abiotic fraction. They assumed that the abiotic rate was directly proportional to the iron sulfide retained for all of the columns in the study. However, the electron microprobe results indicate that the iron sulfides in the column with hematite added (B3) contained two different forms of iron sulfide with vastly different specific surface areas. The framboidal forms, with microcrystal sizes on the order of 1 μm or less had a much higher surface area than the ~10 μm thick coatings on the large ~200 μm iron oxide grains. Therefore, the additional iron sulfide formed by the precipitation of iron sulfide onto the iron oxides (especially magnetite) did not have nearly as much surface area as the framboidal forms that likely existed in all of the columns in roughly equal amounts. The net result of the assumption is an under-prediction of the abiotic contribution to the overall rate.

3.2.2 Compound Specific Isotope Analyses

Carbon stable isotope analysis has been used as a tool to identify biotic and abiotic transformation processes (McKelvie et al., 2007; Liang et al., 2007). Because the bonds between lighter isotopes are easier to break than for the heavier isotopes, the degradation reactions occur faster for chlorinated ethenes containing light isotopes of carbon (^{12}C) than for the heavier isotopes (^{13}C). Therefore, in cases where biotic or abiotic degradation is occurring, the parent compound (TCE or PCE) becomes enriched in ^{13}C (less negative $\delta^{13}\text{C}$ value) in the downgradient groundwater relative to the source area. The degree of enrichment or fractionation that occurs depends on the specific reaction mechanisms that take place during degradation. Thus biotic and abiotic degradation processes may have different isotope fractionation patterns. Discrimination of biotic and abiotic processes was not possible using the carbon stable isotope

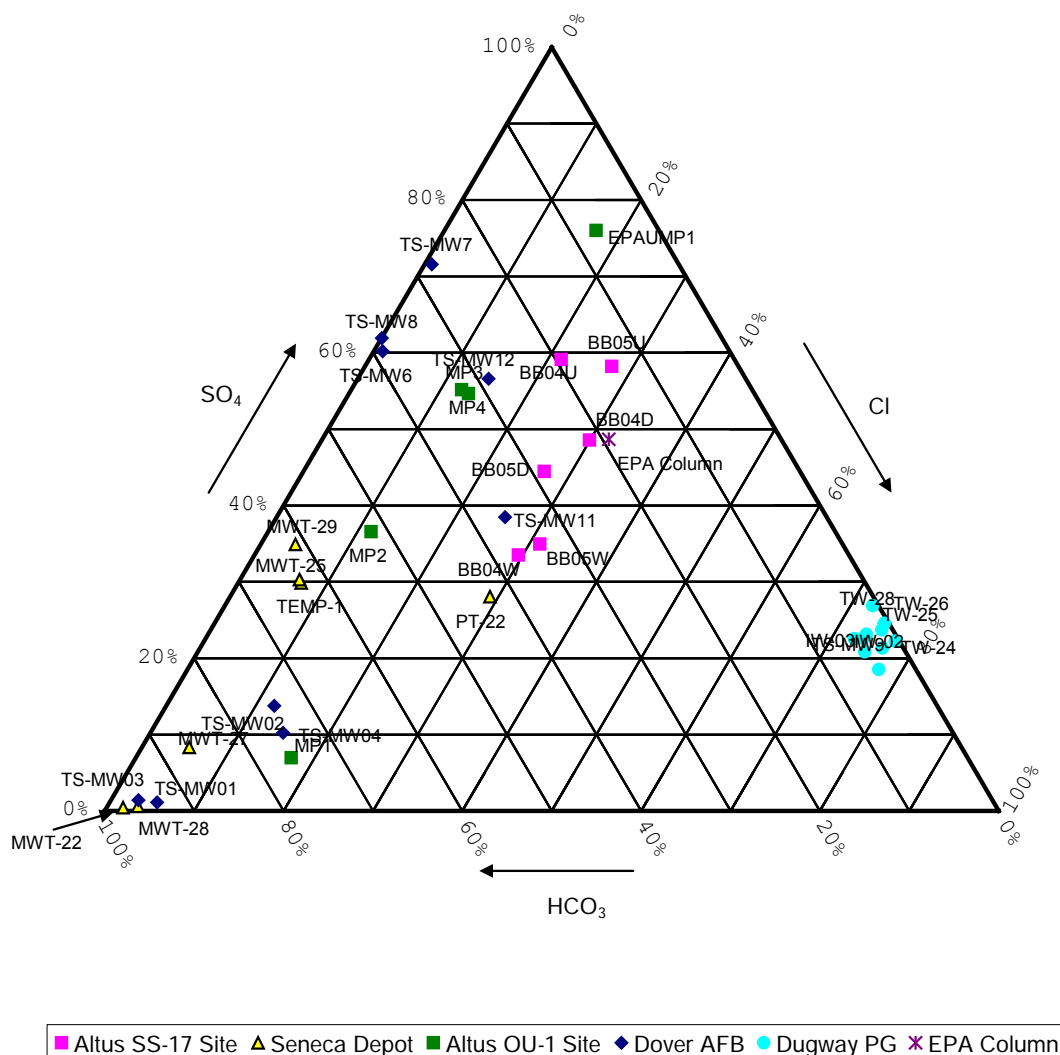


Figure 3-8 – Anion Trilinear Diagram. Some of the labels were intentionally omitted for Dugway Proving Ground due to the tight clustering of the data points. Sample point MWT-26 (Seneca Army Depot Activity) was omitted due to poor charge balance

The Altus AFB SS-17 samples are near the center of both the anion and cations triangles, indicating that the ion mix consists of an approximately equal proportion of ions. The upgradient samples (BB05U and BB04U) have a greater proportion of sulfate compared to the in wall (BB04W and BB05W) and downgradient samples (BB04D and BB05D). The USEPA Column sample, which was generated using the same mulch mix and groundwater as for the SS-17 site at Altus AFB has a similar mix of anions and cations, as it plots within the cluster of pink squares (Altus AFB SS-17) in both figures.

The Dover AFB samples plot along the sulfate-bicarbonate line for the anions and the calcium-magnesium line for the cations, indicating that it is a calcium sulfate-bicarbonate water. The

changes in chemistry may be related to the reactions taking place within the walls. The higher calcium and sulfate fractions (and total concentrations) tend to occur with the area where the gypsum was added (mainly MW08).

The Seneca Army Depot Activity samples ranged from calcium bicarbonate to calcium sulfate. The highest sulfate concentration was in MWT-26 and was anomalously high, but was only slightly elevated above reported background concentrations ranging from 300 to 900 mg/L. For modeling purposes, no bicarbonate was added to achieve charge balance.

The Dugway Proving Ground waters are sodium chloride (sodium was 13,000 to 18,000 mg/L and chloride was 24,500 to 29,800 mg/L) with no apparent variations due to the injection of the organic substrate (vegetable oil) into the aquifer.

The significance of the trilinear diagrams are further discussed during the evaluation of the PHREEQC geochemical modeling.

3.3 Geochemical Equilibrium Modeling

3.3.1 Internal Consistency

The results of the charge and mass evaluations for the groundwater/column data, following the adjustments described in Section 2 are provided in Appendix C. Note that for the waters that were adjusted both a charge balance and mass balance of zero could not be achieved, so the concentrations were adjusted until both the charge balance and mass balance fell within the accepted range of ± 10 percent.

3.3.2 Oxidation-Reduction Potential Evaluation

A summary of the E_h -SHE values (calculated from the platinum electrode field readings) and the E_h determined from the sulfate/sulfide (S(6)/S(-2)) and nitrate/nitrite (N(5)/N(3)) couples are presented in **Table 3-29**. The E_h from the redox couples was calculated by the PHREEQC program using the equation and methodology presented in Appendix C.

Table 3-29 – Summary of E_h Values Calculated Using Different Methods

Site	Sample Identification	Temp. (°C)	E_h -SHE	Sulfate (mg/L)	Sulfide (mg/L)	E_h - S(6)/S(-2) (mV) ^a	E_h - N(5)/N(3) (mV) ^b	Location
Altus AFB OU-1 Site	EPAUMP1	21.8	30.2	2,040	0.005	-172	-	Upgradient
	MP1	20.3	-145.3	145	0.39	-155	-	Within Wall
	MP2	19.4	-84.4	1220	0.59	-152	-	Downgradient
	MP3	20.4	18.6	1480	0.02	-139	-	Downgradient
	MP4	18.7	6.3	1870	0.04	-134	-	Downgradient
Altus AFB SS-17 Site	BB04U	22.1	184.9	1780	0.005	-168	-	Upgradient
	BB04W	22.2	-140.2	1,220	0.42	-176	-	Within Wall
	BB04D	22.5	145.5	1690	0.005	-157	-	Downgradient
	BB05U	22.6	37.4	1560	0.03	-172	-	Upgradient
	BB05W	21.2	-128.2	1290	0.35	-170	-	Within Wall
	BB05D	21.8	36.2	1040	0.01	-152	-	Downgradient

Table 3-29 – Summary of E_h Values Calculated Using Different Methods (cont.)

Site	Sample Identification	Temp. (°C)	E _h -SHE	Sulfate (mg/L)	Sulfide (mg/L)	E _h - S(6)/S(-2) (mV) ^a	E _h - N(5)/N(3) (mV) ^b	Location
Altus AFB SS-17 – USEPA Column	5/15/07	22.3	96	1670	7.55	-224		Column Effluent
Dover AFB – North Transect	TS-MW11	12.5	271.5	6.4	1	-67	-	Upgradient
	TS-MW01	13.6	133.4	3.5	1.3	-120	-	Within UG Wall (North Transect)
	TS-MW02	14.2	305.8	15	1	-91	-	Between Walls
	TS-MW03	13.9	115.1	7.5	1.6	-137	-	Within DG Wall (North Transect)
	TS-MW04	13.3	328.7	9.2	1	-92	-	15 ft Downgradient
Dover AFB – South Transect	TS-MW12	13.1	449.9	34	0.6	-59	-	Upgradient
	TS-MW6	12.5	-3.5	530	3.2	-116.5	-	Within UG Wall (South Transect)
	TS-MW7	13.1	273.9	970	1.3	-102	-	Between Walls
	TS-MW8	13.5	-164.5	1000	51	-131	-	Within DG Wall (South Transect)
	TS-MW9	13.6	331.4	430	0.6	-74	-	15 ft Upgradient
Seneca Army Depot Activity	MWT-25	25	201.5	190	1.3	-215	442	Upgradient
	TEMP-1	25	102.1	180	1.9	-159	461	Within Wall A
	MWT-26	25	236.3	1,000	1.3	-231	426	Downgradient
	MWT-27	25	88	10	0.6	-173	461	Within Wall B1
	MWT-28	25	59.7	3.1	1.6	-172	481	Within Wall B2
	MWT-29	25	286.9	220	1	-182	470	Downgradient
	MWT-22	25	155.3	100	1.6	-185	445	Downgradient
	PT-22	25	148.9	170	1.6	-236	423	Downgradient
Dugway Proving Ground	TW-22	13.8	65.2	11600	0.656	-119	-	Downgradient
	TW-23	13.5	60.5	11200	0.3	-81	-	Downgradient
	TW-24	14.9	447.1	11600	0.003	-47	-	Downgradient
	TW-25	14.78	273.62	12400	0.011	-110	-	Upgradient
	TW-26	13.8	95.2	11900	0.002	-154	-	Crossgradient
	TW-27	14.3	90.7	10900	0.065	-64	-	Crossgradient
	TW-28	13.9	7.1	10,400	1.045	-128	-	Within Injection Zone
	TW-29	13.7	68.3	10800	0.083	-60	-	Downgradient

Notes:

Red Indicates sample from within the main reaction zone (biowall, column, or injection zone)

a) The E_h calculated from the Sulfate/Sulfide redox couple.

b) The E_h calculated from the nitrate/nitrite redox couple.

The ferric/ferrous couple was not used due to the very low aqueous concentrations of ferric iron at low E_h and near-neutral pH. Obtaining ferric iron by difference (subtracting ferrous iron from total iron) could not be performed due to the extremely low concentration of ferric iron in these systems (ferrous and total iron are essentially identical) and the error in the analytical techniques.

A graphical representation of the data is provided in **Figure 3-9** below.

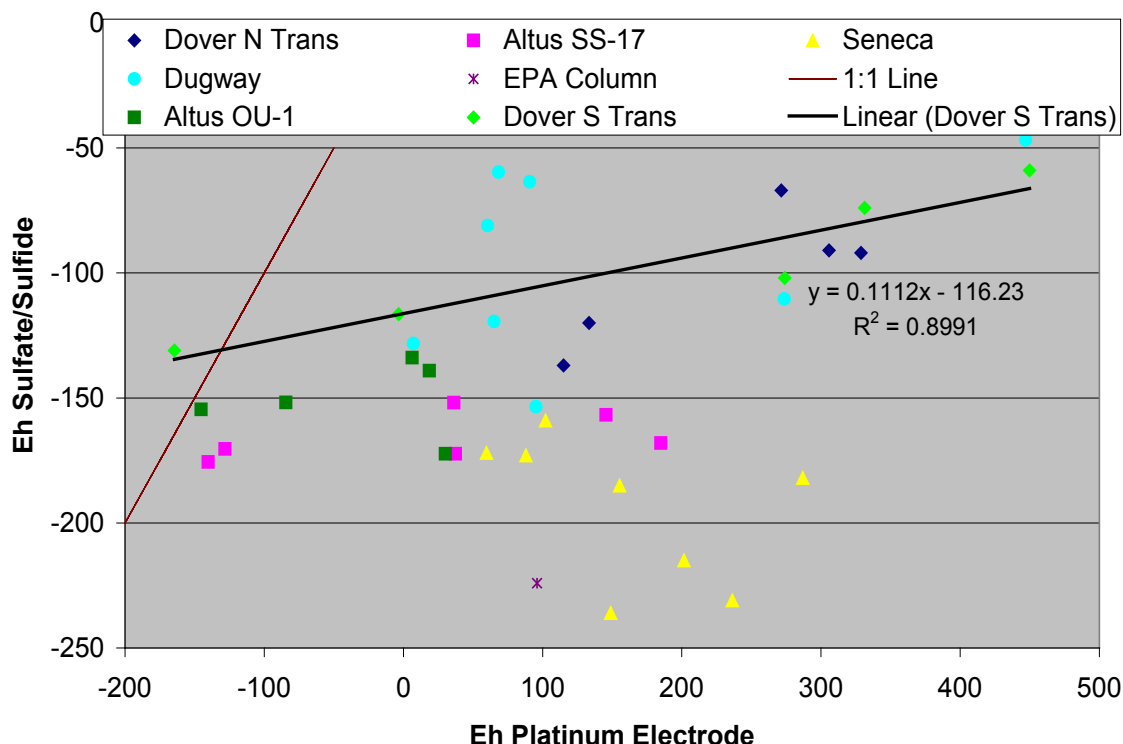


Figure 3-9 - Comparison of the E_h values measured using the platinum electrode (Ag/AgCl_2 reference) with those measured from the sulfate/sulfide redox couple

The fact that nitrate or nitrite is present at all in a system containing sulfide is a strong indication that the system is not in redox equilibrium. Nitrate/nitrite concentrations above the detection limit were reported for the Dover AFB south transect, Altus AFB SS-17 site, and Seneca Army Depot Activity. The one site in which nitrate and nitrite were measured separately (Seneca Army Depot Activity) gave E_h readings between 400 and 500 mV, which contrasts sharply with the sulfide/sulfate couple, which gave E_h readings from -236 mV up to -159 mV. The E_h -SHE for Seneca Army Depot Activity was between these two ranges, with values from 60 mV to 287 mV, suggesting that the platinum electrode (Ag/AgCl_2 reference) was measuring a mixed potential (i.e., the electrode was responding to two or more redox couples at the same time).

Most of the data do not show a correlation, and none follow the 1:1 line as would be expected for a system in redox equilibrium. A linear relationship appears to exist for the Dover AFB South Transect data ($r^2 = 0.90$). The E_h -SHE data have a much broader distribution, reflecting variability in the data.

The lack of redox equilibrium for the waters and the likely mixed potential measured by the platinum electrode precludes the use of E_h -SHE in the model. Because sulfide is the parameter of interest at all of the sites, the E_h used by PHREEQC was set to the sulfate/sulfide couple. Such methodology is consistent with the work of Lindberg and Runnells (1984).

3.3.3 Mineral Saturation States

Iron Minerals

The saturation states of the iron minerals were evaluated to determine which primary minerals may be dissolving (i.e., magnetite, hematite, etc.) under the reducing conditions within the biowalls and to identify which minerals are likely to be precipitating as a result of the biological and abiotic reactions occurring within the biowalls (i.e., iron monosulfides, green rust, or sedimentary magnetite). The results of the PHREEQC modeling for the iron minerals are provided in **Tables 3-30** through **3-36**.

The tables express the saturation state by means of a saturation index (SI), which is defined using Equation 2-1. The tables do not include the SI values for the several green rust phases that were modeled, because all of them (with the exception of one phase which was always supersaturated and is considered to be based on inaccurate thermodynamic data) were undersaturated in all of the solutions modeled. The iron sulfide mineral greigite was also undersaturated in most of the samples and was only included in the summary tables when the phase was at or near saturation for one or more of the samples from that site. The high pH mackinawite phase investigated by Rickard (2006) which has been named “alkaline mackinawite” for the purposes of this report was only included for sites which had pH values greater than 7 (Seneca Army Depot Activity and USEPA column).

OU-1 Site

The OU-1 site samples are generally saturated with respect to the iron monosulfides troilite and mackinawite (**Table 3-30**). The slight supersaturation of troilite may be due to compositional variations. The troilite thermodynamic data are based on the pure stoichiometric phase with the formula FeS. However, in nature there are often vacancies in the structure where Fe^{+2} atoms are missing. In order to maintain charge balance some of the Fe^{+2} atoms are replaced by Fe^{+3} atoms. When vacancies are present, the mineral is referred to as pyrrhotite and has the general formula $(Fe^{+2}_{1-3x}Fe^{+3}_{2x}S)$ where x is the fraction of vacancies in the structure. For each value of x, the solubility changes, such that it would be a very difficult phase to model. However, the fact that troilite, which is the form without vacancies (x=0) is close to saturation suggests that pyrrhotite phases are probably close to saturation as well and could be at saturation. The iron monosulfide mineral marcasite is also either at or very close to saturation. As with the SS-17 samples, the electron microprobe results indicated that the iron sulfides present were iron disulfides, while the AVS/CrRS results showed a mixture of the two. Again, iron disulfide appears to be formed from the alteration of iron monosulfides (in this case troilite and possibly mackinawite) to iron disulfides. Anderko and Shuler (1997) evaluated thermodynamic information and experimental data from other investigators to obtain the following alteration sequence for the iron monosulfides:

mackinawite (poorly ordered) → mackinawite (crystalline) → troilite (or pyrrhotite)

Therefore, it is possible that the first formed phase was poorly ordered mackinawite, which has since altered to either crystalline mackinawite or troilite with subsequent equilibration of the solution with one or both of these minerals.

The iron disulfide present could be either pyrite or marcasite. Anderko and Shuler (1997) list the alteration sequence for the iron disulfides as:

marcasite → *pyrite*

However, the solution did not equilibrate with either of these phases (despite the fact that one or both are present) due to kinetic inhibitions.

Table 3-30 - Summary of Saturation Index Values Calculated Using PHREEQC - Altus AFB OU-1 Site

Sample Identification	Type	Poorly Ordered Crystalline Mackinawite	Mackinawite	Magnetite	Marcasite	Pyrite	Troilite
		FeS	FeS	Fe ₃ O ₄	FeS ₂	FeS ₂	FeS
EPAUMP1	UG	-1.95	-1.21	-12.85	5.92	6.65	0.33
MP1	W	-1.19	-0.45	-13.96	8.34	9.07	1.1
MP2	DG	-1.32	-0.58	-17.92	8.58	9.31	0.98
MP3	DG	-1.54	-0.8	-13.89	7.26	7.98	0.75
MP4	DG	-2.06	-1.32	-13.28	6.4	7.13	0.24

Notes:

Shading indicates mineral saturation given the criteria of Hem (1970) of SI = 0 ±0.5 (rounded).

DG - downgradient.

UG - upgradient.

W - within wall.

Two sulfur deficient iron disulfide grains were found in the Altus AFB OU-1 samples (see Appendix D, Attachment 1) during the electron microprobe analysis (C1-A grain 1 with 48.7 percent sulfur and C6-A grain 7 with 46.6 percent sulfur). Pure stoichiometric iron disulfide would have 53.5 percent sulfur. These results suggest that the conversion of iron monosulfide to iron disulfide or greigite was incomplete.

SS-17 Site

The Altus AFB samples collected from the SS-17 site, upgradient, downgradient, and within the walls all appear to be saturated with respect to the iron monosulfide mineral troilite (**Table 3-31**).

Table 3-31 – Summary of Saturation Index Values Calculated Using PHREEQC – Altus AFB SS-17 Site

Sample Identification	Type	Poorly Ordered Crystalline Mackinawite	Mackinawite	Magnetite	Marcasite	Pyrite	Troilite
		FeS	FeS	Fe ₃ O ₄	FeS ₂	FeS ₂	FeS
SS-17 Site							
BB04U	UG	-2.5	-1.76	-14.62	5.4	6.12	-0.22
BB04W	W	-2.47	-1.74	-20.98	6.92	7.64	-0.2
BB04D	DG	-2.73	-1.99	-15.54	5.28	6	-0.46
BB05U	UG	-2.07	-1.33	-15.97	6.41	7.13	0.2
BB05W	W	-2.68	-1.94	-21.27	6.76	7.48	-0.4
BB05D	DG	-2.06	-1.32	-14.57	6.27	6.99	0.22

Notes:

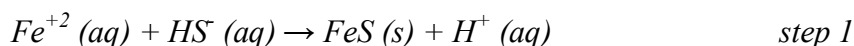
Shading indicates mineral saturation given the criteria of Hem (1970) of SI = 0 ±0.5 (rounded).

DG - downgradient.

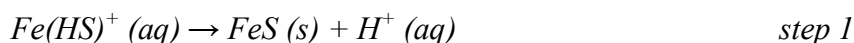
UG - upgradient.

W - within wall.

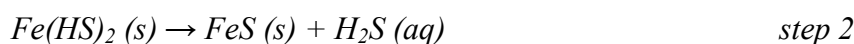
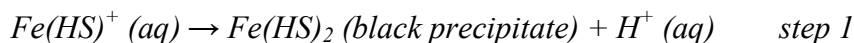
The iron disulfide minerals pyrite and marcasite are both supersaturated (SI>0.5), which indicates that these minerals are thermodynamically predicted to precipitate, but have not precipitated due to kinetic limitations. The kinetic inhibition to the precipitation of iron disulfides is well documented (summarized in Wei and Osseo-Asare, 1995; Anderko and Shuler, 1997). Iron disulfides such as pyrite and marcasite do form at low temperature, but as an alteration product of iron monosulfides and not as a direct precipitate. Pyrite is thought to form by a two-step process (13 references cited by Wei and Osseo-Assare, 1995) as follows:



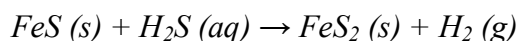
Based on their spectrophotometric analysis, Wei and Osseo-Assare (1995) propose the following two step process for the formation of iron disulfide:



or alternatively, the three step process;



The undersaturation with respect to native sulfur (S^0) determined from the PHREEQC modeling suggests that reaction between iron monosulfides and native sulfur is unlikely, except perhaps within microenvironments such as on mineral surfaces. Rickard (1997) proposed hydrogen sulfide as the primary oxidant resulting in the conversion of iron monosulfide to iron disulfide. The proposed reaction is as follows:



The reaction is very rapid and is pH dependant, with faster reaction rates at lower pH.

Another possibility is that iron monosulfides are converted to iron disulfides as a result of the reductive dechlorination of chlorinated ethenes. In this case, sulfide would be the electron donor. Such a reaction was shown to be thermodynamically possible by Haas and Shock (1999).

Based on the modeling results presented above, the initial phase formed in the SS-17 samples was FeS (troilite). However, the electron microprobe results did not identify any iron sulfide phases, while the AVS/CrRS results showed a mixture of iron disulfide and iron monosulfide. The sample likely contains iron sulfides of different ages that are in various stages of alteration from iron monosulfide to iron disulfide. Wei and Osseo-Assare (1995) state that sulfur deficiencies up to seven percent in pyrite may be caused by the formation of iron disulfide around a core of iron monosulfide.

Other minerals or phases were undersaturated ($SI < -0.5$), which means that they would not be expected to precipitate from solution, or if already present in the mulch as a primary mineral, they would be expected to dissolve. However, if a mineral is present and is undersaturated, it suggests that the phase is not in equilibrium. Under equilibrium conditions, the mineral would dissolve until the solution is saturated with respect to that mineral and equilibrium is established. Magnetite and hematite (not shown in table) are examples of phases that were present in the samples, but were consistently predicted to be undersaturated in the groundwater.

USEPA Column Study (SS-17 Site)

The column effluent sample was at saturation with respect to poorly ordered crystalline mackinawite (Table 3-32).

Table 3-32 - Summary of Saturation Index Values Calculated Using PHREEQC – USEPA Column Study (Altus AFB Site SS-17)

Sample Id	Poorly Ordered Crystalline Mackinawite	Crystalline Mackinawite	Alkaline Mackinawite ^a	Magnetite	Hematite	Marcasite	Pyrite	Troilite
	FeS	FeS	FeS	Fe ₃ O ₄	Fe ₂ O ₃	FeS ₂	FeS ₂	FeS
Col B3	-0.12	0.62	-0.79	-17.15	-0.91	9.69	10.41	2.16

Notes:

Shading indicates mineral saturation given the criteria of Hem (1970) of $SI = 0 \pm 0.5$ (rounded).

a) Phase solubility determined by Rickard (2006), “alkaline” refers to form of mackinawite formed at $pH > 7$.

Both hematite and magnetite were undersaturated, although hematite was close to saturation. The

model predicts that both hematite and magnetite would dissolve within the solution. The residence time in the columns (17 days) may not have been long enough for crystalline forms of the minerals to dissolve to the point of saturation. Reaction rates were also likely limited by coatings of other phases onto these minerals (see electron microprobe results). The ions dissolved from the phase would have to diffuse through the surface coating before additional dissolution would occur, which would make diffusion the rate-limiting step.

Dover AFB

The Dover AFB samples were generally at saturation with respect to the iron monosulfides poorly ordered mackinawite, crystalline mackinawite, or troilite (**Table 3-33**). The exception was for wells TMW-04 and TMW-12, which were undersaturated for all of the iron monosulfides.

Table 3-33 - Summary of Saturation Index Values Calculated Using PHREEQC - Dover AFB

Sample ID	Type	Poorly Ordered Crystalline Mackinawite	Crystalline Mackinawite	Magnetite	Marcasite	Pyrite	Troilite
		FeS	FeS	Fe ₃ O ₄	FeS ₂	FeS ₂	FeS
TS-MW11	UG	-2.42	-1.66	-9.99	18.51	19.26	-0.06
TS-MW01	UG	-0.6	0.16	-4.5	22	22.74	1.75
TS-MW02	BW	-1.29	-0.53	-7.01	20.52	21.26	1.06
TS-MW03	W	-0.23	0.53	-3.11	22.92	23.67	2.12
TS-MW04	DG	-3.86	-3.1	-14.64	17.98	18.73	-1.51
TS-MW12	UG	-4.81	-4.05	-17.59	16.07	16.81	-2.46
TS-MW06	W	-0.08	0.68	-3.71	23.19	23.94	2.28
TS-MW07	BW	-1.11	-0.35	-6.06	21.44	22.19	1.24
TS-MW08	BW	-0.61	0.15	-8.86	23.96	24.71	1.74
TS-MW09	DG	-1.83	-1.07	-8.1	19.61	20.35	0.52

Notes:

Shading indicates mineral saturation given the criteria of Hem (1970) of SI = 0 ±0.5 (rounded).

DG – downgradient.

UG - upgradient.

W - within wall.

BW - between walls.

Seneca Army Depot Activity

The Seneca Army Depot Activity samples were either not at saturation with respect to any iron sulfide minerals evaluated or were at saturation with one of the iron monosulfides (**Table 3-34**).

Table 3-34 – Summary of Saturated Index Values Calculated Using PHREEQC – Seneca Army Depot Activity

Sample ID	Type	Poorly Ordered Crystalline Mackinawite	Mackinawite (Alkaline Conditions) ^a	Greigite	Magnetite	Marcasite	Pyrite	Troilite
		FeS	FeS	Fe ₃ S ₄	Fe ₃ O ₄	FeS ₂	FeS ₂	FeS
MWT-25	UG	-0.16	-0.81	-4.81	-15.61	8.92	9.64	2.09
TEMP-1	W	1.17	0.62	0.15	-12.56	10.95	11.66	3.42
MWT-26	BW	-0.04	-0.80	-5.00	-14.09	8.8	9.51	2.21
MWT-27	BW	1.59	0.74	-0.62	-9.6	10.46	11.17	3.84
MWT-28	W	1.14	0.59	-0.45	-12.87	10.41	11.13	3.39
MWT-29	DG	-0.63	-1.15	-5.48	-17.2	8.78	9.5	1.62
MWT-22	DG	1.09	0.51	-0.53	-12.58	10.5	11.22	3.34
PT-22	BW	0.85	0.07	-2.43	-12.31	9.67	10.38	3.1

Notes:

Shading indicates mineral saturation given the criteria of Hem (1970) of SI = 0 ±0.5 (rounded).

a) Phase solubility determined by Rickard (2006), “alkaline” refers to form of mackinawite formed at pH>7.

DG – downgradient.

UG – upgradient.

W - within wall.

BW - between walls.

Poorly ordered mackinawite was supersaturated for all of the samples, except for downgradient sample MWT-29, upgradient samples MWT-25, and between walls sample MWT-26. Because mackinawite precipitation is generally not kinetically inhibited, the supersaturation may be due to the presence of mackinawite nanoparticles within the solution which passed through the 0.45 µm filter and was included within the dissolved analysis. The ionic strength of the Seneca Army Depot Activity “in-wall” water samples ranged from 0.017 to 0.034 molar, which is an order of magnitude lower than the ionic strength used by Rickard (2006) (0.1 molar) to coagulate mackinawite nanoparticles. Therefore, if nanoparticles were present in the water samples it would not have coagulated and collected on the filters, but instead would have been included as part of the “dissolved” analysis.

Another possibility is that the pH of some of the Seneca Army Depot Activity groundwaters (6.35 to 7.46) were high enough to create mackinawite from “aqueous clusters”, which take the form Fe_nS_n⁰ where n is either 2 or 4 (cited in Rickard, 2006). At pH values greater than 7, the cluster complex becomes the dominant form of aqueous iron in solution (surpassing Fe⁺²). The intrinsic stability constant of the cluster complex provided by Rickard (2006) was entered into the PHREEQC database (as FeS⁰). The sample with the highest pH (PT-22 with a pH of 7.46) was also at saturation with “alkaline mackinawite” and the dissolved ferrous iron was dominated by the cluster complex (50 percent FeS⁰ on a molar basis), in agreement with the findings of Rickard (2006). Therefore, it is likely that the slightly more soluble form of mackinawite which is formed at pH>7 is the precipitating iron sulfide within these samples. The in-wall samples were either at saturation with respect to greigite (TEMP-1 and MWT-28), or slightly supersaturated with respect to alkaline mackinawite (MWT-27 and MWT-28). Because greigite does not form directly from solution, saturation with respect to this mineral would have resulted from aging of mackinawite (Butler and Hayes, 2001), and/or oxidation, possibly by chlorinated ethenes. The

saturation with (or near saturation) with respect to alkaline mackinawite suggests that the highly reactive poorly ordered mackinawite nanoparticles are not present in solution.

Dugway Proving Ground

The Dugway samples were either undersaturated with respect to the iron sulfides or were at saturation with respect to one of the iron monosulfide phases (**Table 3-35**).

Table 3-35 - Summary of Saturation Index Values Calculated Using PHREEQC - Dugway Proving Ground

Sample ID	Type	Poorly ordered crystalline Mackinawite	Crystalline Mackinawite	Magnetite	Marcasite	Pyrite	Troilite
		FeS	FeS	Fe ₃ O ₄	FeS ₂	FeS ₂	FeS
TW-22	DG	-0.43	0.33	-14.87	10.26	11	1.92
TW-23	DG	-1.53	-0.77	-17.05	9.22	9.97	0.82
TW-24	DG	-6.53	-5.77	-25.61	2.81	3.55	-4.19
TW-25	UG	-3.96	-3.21	-19.83	5.3	6.05	-1.63
TW-26	CG	-2.68	-1.92	-12.86	5.51	6.25	-0.33
TW-27	CG	-2.68	-1.92	-12.86	5.51	6.25	-0.33
TW-28	Inj	-0.35	0.41	-15.29	10.4	11.14	1.99
TW-29	DG	-2.39	-1.63	-17.75	8.06	8.8	-0.04

Notes:

Shading indicates mineral saturation given the criteria of Hem (1970) of SI = 0 ±0.5 (rounded).

DG - downgradient.

UG - upgradient.

CG - crossgradient.

Inj - injection zone.

Summary of Saturated Reduced Iron Phases by Site

A summary of the reduced-iron phases by site is presented in **Table 3-36**.

Table 3-36 – Summary of Saturated Reduced-Iron Phases by Site

Site	Reduced-Iron Phases at Saturation
Altus AFB OU-1	Troilite (FeS)/Mackinawite (FeS _{1-x})
Altus AFB SS-17	Troilite (FeS)
Altus AFB SS-17 (USEPA Column)	Poorly ordered mackinawite (FeS _{1-x})
Dover AFB – North Transect	Troilite (FeS)/Crystalline mackinawite (FeS _{1-x})
Dover AFB – South Transect	Poorly ordered mackinawite (FeS _{1-x}) /Crystalline mackinawite (FeS _{1-x})
Seneca Army Depot Activity	Poorly ordered mackinawite (FeS _{1-x}) /Alkaline mackinawite (FeS _{1-x})/Greigite (Fe ₃ S ₄)
Dugway Proving Ground	Poorly ordered mackinawite (FeS _{1-x}) /Crystalline mackinawite (FeS _{1-x})/Troilite (FeS)

Sulfate Phases and Calcite

The saturation states of the sulfate and calcium phases were evaluated in order to determine what reactions likely control the sulfate concentrations within the biowalls and aquifer materials. Sulfate is important as an electron acceptor for sulfate-reducing bacteria. Sulfate loadings in and out of a bioreactor are often used to determine the rate of sulfate reduction within the system. However, when minerals such as gypsum ($\text{CaSO}_4 \cdot 2 \text{H}_2\text{O}$), anhydrite (CaSO_4), and barite (BaSO_4) are present within the biowall or aquifer matrix, dissolution reactions can occur in response to the removal of sulfate from the solution (by formation of sulfide and precipitation as iron sulfide minerals). Such mineral dissolution can make the sulfide production rate to appear to be lower than it really is (because the sulfate in versus sulfate out mass balance to determine sulfide formed becomes invalid). Sulfate minerals can also precipitate within the system, making the degree of sulfate reduction appear to be greater than it really is. In order to evaluate if dissolution/precipitation reactions are occurring in either the biowalls or the aquifer, the saturation state of the sulfate minerals were evaluated. The mineral calcite was also evaluated, as aqueous calcium concentrations control the solubility of gypsum and anhydrite. For example, water which is undersaturated with respect to gypsum within the aquifer may reach saturation by coming into contact with calcite existing in the biowall or as part of the site lithology (i.e., a limestone layer). The calcite would dissolve, which would increase the calcium in solution until both calcite and gypsum have reached saturation (gypsum is slightly less soluble than anhydrite). Therefore, the saturation state of calcite was also evaluated.

The results of the PHREEQC modeling for the sulfate minerals and calcite are presented in **Tables 3-37** through **3-42**.

OU-1 Site

The OU-1 site exhibits nearly the exact same pattern as for SS-17 (see below), which is not surprising considering that both sites are located within the same hydrogeologic unit. In this case, the undersaturation of gypsum within the wall (sample MP-1) is more pronounced (for SS-17 the two wall samples would be considered saturated, but the SI values are lower than for the upgradient and downgradient samples for the most part).

Table 3-37 - Summary of Saturation Index Values for Selected Calcium and Sulfate Minerals Calculated Using PHREEQC - Altus AFB OU-1 Site

Sample Id	Type	Gypsum	Anhydrite	Barite	Calcite	Notes
		$\text{CaSO}_4 \cdot 2 \text{H}_2\text{O}$	CaSO_4	BaSO_4	CaCO_3	
EPAUMP1	UG	-0.06	-0.29	-0.11	0.11	Same lithology as SS-17. Northern part of wall receives reducing water from the Landfill 3 bioreactor
MP1	W	-1.21	-1.45	1	0.46	
MP2	DG	-0.16	-0.4	1.14	0.73	
MP3	DG	-0.14	-0.38	0.15	0.31	
MP4	DG	-0.08	-0.32	0.03	0.39	

Notes:

DG – downgradient.

UG – upgradient.

W - within wall.

The distribution of the points on the anion trilinear diagram also show the same pattern, with sulfate-rich upgradient samples, bicarbonate-rich wall samples, and downgradient samples with an intermediate composition. Therefore, the interpretation for the OU-1 site is the same as for SS-17 in terms of the reactions involving gypsum, barite, and calcite.

SS-17 Site

Gypsum, barite, and calcite are either at saturation or slightly supersaturated in all of the groundwaters, with the exception of BB05D, which is very close to saturation with respect to gypsum (Table 3-38).

Table 3-38 - Summary of Saturation Index Values for Selected Calcium and Sulfate Minerals Calculated Using PHREEQC - Altus AFB SS-17 Site

Sample Identification	Type	Gypsum CaSO ₄ · 2 H ₂ O	Anhydrite CaSO ₄	Barite BaSO ₄	Calcite CaCO ₃	Notes
BB04U	UG	-0.31	-0.54	-0.1	0.22	Weathered and fractured silty clay extends to a depth of approximately 25 to 30 feet bgs, which is underlain by silt and dense shale of the Hennessey Group
BB04W	W	-0.49	-0.72	1.04	0.53	
BB04D	DG	-0.32	-0.55	-0.14	0.3	
BB05U	UG	-0.49	-0.72	-0.11	0.11	
BB05W	W	-0.46	-0.69	1.17	0.57	
BB05D	DG	-0.6	-0.83	0.29	0.04	

Notes:

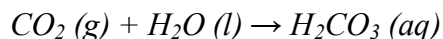
DG – downgradient.

UG – upgradient.

W - within wall.

The presence of gypsum and barite within the aquifer matrix would explain the replenishment of sulfate observed within wells downgradient of the biowall (Parsons, 2008). The saturation with respect to calcite could be due either to precipitation of the mineral from solution or by dissolution of limestone within the biowall or cements within the aquifer matrix. In the case of the SS-17 calcite is likely present in the aquifer, as the upgradient samples are at saturation. Precipitation of calcite is likely occurring within the biowall and within the down-gradient aquifer (adding to the calcite already present).

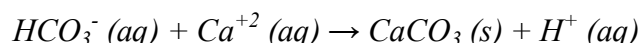
Precipitation of calcite from a solution saturated with respect to gypsum could occur within the biowall by the production of alkalinity resulting from the mineralization of organic matter by bacteria. The carbon dioxide produced would combine with water to form carbonic acid as follows:



Which dissociates to bicarbonate at near neutral pH (assuming the system is well buffered) as follows:



The bicarbonate then combines with the calcium in solution (provided by dissolution of gypsum within the aquifer) to form calcite as follows:



The consumption of sulfate within the wall by the sulfate-reducing bacteria would result in the temporary undersaturation of gypsum. However, when the water comes into contact with gypsum within the downgradient aquifer dissolution would occur until gypsum saturation is reached. However, due to the increased bicarbonate added within the biowall the increased calcium resulting from the gypsum dissolution would supersaturate the system with respect to calcite, resulting in precipitation of calcite (adding to the calcite already present within the aquifer). Such a process would explain the trend in the anion trilinear diagram (presented above) in which the upgradient waters have the lowest fraction of bicarbonate relative to sulfate, and the biowall waters have the highest (with the downgradient samples in an intermediate position). The production of alkalinity in the wall and the simultaneous removal of sulfate (by the sulfate-reducing bacteria) is the reason that the wall samples have the highest bicarbonate fraction. The precipitation of calcite and dissolution of gypsum downgradient results in the higher sulfate fraction, but not as high as in the upgradient groundwater.

SS-17 (USEPA Column)

The USEPA column effluent appears to have been saturated with respect to gypsum and slightly supersaturated with respect to calcite and barite (**Table 3-39**).

Table 3-39 - Summary of Saturation Index Values for Selected Calcium and Sulfate Minerals Calculated Using PHREEQC - USEPA Column (Altus AFB Site SS-17)

Sample Identification	Type	Gypsum	Anhydrite	Barite	Calcite	Notes
		$\text{CaSO}_4 \cdot 2 \text{H}_2\text{O}$	CaSO_4	BaSO_4	CaCO_3	
Col B3	Effluent	-0.26	-0.49	1.06	0.95	Column contained the SS-17 mulch mixture with added hematite (but not limestone)

Production of carbon dioxide gas in the column likely resulted in an increase in alkalinity and precipitation of calcite. On the trilinear diagram, the USEPA column effluent sample plots nearly on top of the downgradient sample BB04D at the SS-17 site. The fact that calcite is likely precipitating within the column explains why the column with hematite and limestone added did not perform any better than the sample with only hematite added. The limestone would be essentially inert in an environment where calcite is precipitating (i.e., limestone cannot dissolve when calcite is at saturation).

Dover AFB

The Dover AFB samples are undersaturated with respect to gypsum, anhydrite, and calcite, with the exception of the samples collected from the area where gypsum was added (**Table 3-40**).

Table 3-40 - Summary of Saturation Index Values for Selected Calcium and Sulfate Minerals Calculated Using PHREEQC - Dover AFB

Sample Id	Type	Gypsum	Anhydrite	Barite	Calcite	Notes
		$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$	CaSO_4	BaSO_4	CaCO_3	
TS-MW11	UG	-3.8	-4.06	NA ^a	-4.34	North Transect
TS-MW01	W _{UG}	-3.16	-3.42	NA ^a	-1.45	
TS-MW02	BW	-2.93	-3.18	NA ^a	-2.8	
TS-MW03	W _{DG}	-2.58	-2.83	NA ^a	-0.63	
TS-MW04	DG	-3.25	-3.5	NA ^a	-3.01	South Transect - Powdered gypsum added to the southern sections of both walls
TS-MW12	UG	-2.8	-3.05	NA ^a	-4.11	
TS-MW06	W _{UG}	-0.7	-0.95	NA ^a	-0.89	
TS-MW07	BW	-0.22	-0.47	NA ^a	-0.69	
TS-MW08	W _{DG}	-0.02	-0.27	NA ^a	0.08	
TS-MW09	DG	-1	-1.25	NA ^a	-3.74	

Notes:

a) No barium analyses were available.

DG - downgradient.

UG - upgradient.

W_{UG} - within upgradient wall.

W_{DG} - within downgradient wall.

BW - between walls.

Neither gypsum nor calcite appears to be present within the aquifer matrix. Calcite is not at saturation within the non-gypsum amended wall samples (North Transect), even with the alkalinity addition taking place there (from biodegradation of organic carbon to carbon dioxide), due to relatively low calcium concentrations in the groundwater. The fact that limestone was part of the mulch mixture (**Table 1-1**) would imply that calcite should be saturated within the wall, especially given the long residence time within the biowalls.

Not surprisingly, gypsum is at saturation for the samples collected from the area where powdered gypsum was amended to the mulch mix (TS-MW07 and TS-MW-08). In this area, calcite is either at saturation or close to saturation due to the simultaneous addition of calcium (from gypsum dissolution) and alkalinity production (from mineralization of organic matter).

Seneca Army Depot Activity

The Seneca Army Depot Activity samples are generally saturated or supersaturated with respect to calcite and undersaturated with respect to gypsum and anhydrite (with the exception of MWT-26 which is saturated with respect to gypsum) as shown in **Table 3-41**.

Table 3-41 – Summary of Saturation Index Values for Selected Calcium and Sulfate Minerals Calculated Using PHREEQC – Seneca Army Depot Activity

Sample Identification	Type	Gypsum	Anhydrite	Barite	Calcite	Notes
		$\text{CaSO}_4 \cdot 2 \text{H}_2\text{O}$	CaSO_4	BaSO_4	CaCO_3	
MWT-25	UG	-1.19	-1.41	NA ^a	0.65	
TEMP-1	W	-1.15	-1.37	NA ^a	-0.31	In biowall A
MWT-26	BW	-0.5	-0.72	NA ^a	0.72	
MWT-27	W	-2.21	-2.43	NA ^a	NA ^b	In biowall B1
MWT-28	W	-2.91	-3.13	NA ^a	0.32	In biowall B2
MWT-29	DG	-1.13	-1.35	NA ^a	0.2	
MWT-22	DG	-1.27	-1.49	NA ^a	0.23	
PT-22	BW	-1.36	-1.58	NA ^a	1.01	

Notes:

a) No barium analyses were available.

b) No alkalinity data were available.

W - within wall.

BW - between walls.

The reason that sample MWT-26 is saturated with gypsum is attributable to its anomalously high sulfate concentration (see Section 3.2.3).

The conclusion is that the aquifer likely contains calcite. Alkalinity production within the walls likely results in precipitation of calcite within the mulch. The most undersaturated samples with respect to gypsum are wall samples MWT-28 (biowall B2) and MWT-27 (biowall B1), suggesting that sulfate reduction is taking place within the walls.

Dugway Proving Ground

All of the Dugway Proving Ground samples are saturated with respect to gypsum and anhydrite and close to or at saturation with respect to calcite (**Table 3-42**)

Table 3-42 - Summary of Saturation Index Values for Selected Calcium and Sulfate Minerals Calculated Using PHREEQC - Dugway Proving Ground

Sample Id	Type	Gypsum	Anhydrite	Barite	Calcite
		$\text{CaSO}_4 \cdot 2 \text{H}_2\text{O}$	CaSO_4	BaSO_4	CaCO_3
TW-22	DG	0.16	-0.07	NA ^a	-0.45
TW-23	DG	0.12	-0.1	NA ^a	-0.64
TW-24	DG	0.09	-0.13	NA ^a	-1.68
TW-25	UG	0.11	-0.11	NA ^a	-0.76
TW-26	CG	0.11	-0.28	NA ^a	-0.13
TW-27	CG	0.06	-0.16	NA ^a	-0.78
TW-28	Inj	0.04	-0.17	NA ^a	0.17
TW-29	DG	0.06	-0.17	NA ^a	-0.78

Note:

a) No barium analyses were available.

There is no apparent change in gypsum saturation within or downgradient of the injection zone, suggesting that sulfate reduction is minimal. The Dugway samples plot in very tight clusters near the sodium plus potassium and chloride portions of the trilinear diagrams, suggesting that the upgradient, injection zone, and downgradient waters are essentially identical in terms of major ion chemistry. The groundwater in the area may be influenced by evaporate deposits, which typically contain sequences of limestone, gypsum, and halite (NaCl), or by connate brines.

Summary of Calcite and Gypsum Saturation by Site

A summary of the gypsum, barite, and calcite saturation states are shown in **Table 3-43**.

Table 3-43 – Summary of Calcite, Gypsum and Barite Saturation by Site

Site	Phases at Saturation
Altus AFB OU-1	Barite (BaSO_4), calcite (CaCO_3), anhydrite (CaSO_4), and gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$)
Altus AFB SS-17	Barite (BaSO_4), calcite (CaCO_3), and gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$)
Altus AFB SS-17 (USEPA Column)	Anhydrite (CaSO_4) and gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$) saturated; Barite (BaSO_4) and calcite (CaCO_3) supersaturated
Dover AFB – North Transect	None
Dover AFB – South Transect	Anhydrite (CaSO_4), gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$) and calcite (CaCO_3)
Seneca Army Depot Activity	Calcite (CaCO_3) ^a
Dugway Proving Ground	Anhydrite (CaSO_4), gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$) and calcite (CaCO_3)

Note:

- a) Gypsum was at saturation for MWT-26. However, the sulfate analysis was unusually high (based on charge balance and mass balance evaluations).

4.0 Summary and Interpretation

4.1 Parameters Affecting Abiotic Dechlorination

Based on the results of this investigation and the results reported in the literature, the parameters listed in **Table 4-1** appear to be the most important variables in evaluating success factors for *in situ* abiotic dechlorination-based treatment systems.

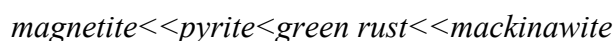
Table 4-1 – Summary of Parameters Affecting *In Situ* Biogeochemical Transformation of Chlorinated Ethenes

Parameter	Optimal
Reduced iron phase mineralogy	Freshly formed iron monosulfides and disulfides.
Iron sulfide surface area	High to increase reaction rates.
E _h /pH conditions of the water	pH>6 since iron sulfide reactivity increases with pH, E _h <100 mV to promote formation or reactive iron sulfides.
Volumetric sulfate loading rate	High to ensure constant renewal of reactive iron sulfides. Is accomplished through a combination of sulfate concentration and hydraulics necessary to generate a dynamic system.
Ionic strength	Sufficiently low to prevent coagulation of nanoparticulate iron sulfide and reduction of reactive mineral surface area.
Organic carbon content of the solid media (mulch or vegetable oil) and dissolved organic carbon	Sufficiently high to provide high rates of biological sulfate reduction and to prevent influx of dissolved oxygen.
Dissolved oxygen	Minimized infiltration of dissolved oxygen via groundwater flow or surface water infiltration
Iron oxide mineral surface area and availability	High to provide a source of iron for reactive iron sulfide formation.

Each factor is described in detail in the following subsections, while an assessment of each system with regard to each of these parameters and the relative success of each is presented in Section 4.2.

4.1.1 Reduced Iron Phase Mineralogy

The rate of reaction between chlorinated ethenes and reduced iron phases is very much dependant on the mineral phases present, the degree of crystallinity, and even the age of the phases. Lee and Batchelor (2002a) determined that the surface area-normalized pseudo-first order rate constant (rate constant divided by the surface area of the mineral) for pyrite was 23.5 to 40.3 times greater than for magnetite, while Lee and Batchelor (2002b) determined that the same rate constant for green rust was 3.4 to 8.2 times that for pyrite. Rate constants calculated by Butler and Hayes (1999 and 2001) suggest that the rate of iron monosulfides are even faster than for green rusts. Therefore, the overall order of reactivity for the common reduced iron phases is as follows:



However, the relatively low surface area-normalized rate constant for pyrite compared to mackinawite may be due to the fact that Lee and Batchelor (2002a) used coarse crystalline pyrite (ground to 63 to 250 μm diameter), whereas Butler and Hayes (1999 and 2001) used freshly precipitated mackinawite. In addition, the specific surface area measured by Lee and Batchelor (2002a) of 27.8 m^2/g appears to be an order of magnitude too high compared to other measurements (see discussion below). Therefore, pyrite probably has a higher surface area-normalized rate constant than green rust. The rate data obtained by Weerasooriya and Dharmasena (2001) for TCE abiotic degradation by pyrite would seem to confirm this. According to Elsner et al. (2004) the abiotic degradation rate constant of other chlorinated compounds such as 4-chloronitrobenzene, 4-chlorophenyl hydroxylamine, and hexachloroethane in the presence of adsorbed ferrous iron follows the order:

$$\text{Siderite} < \text{magnetite} < \text{green rust} < \text{pyrite} < \text{mackinawite}$$

As green rusts could not be identified conclusively and very few iron oxyhydroxides with a composition consistent with green rusts were identified during the electron microprobe analysis, green rusts are not considered important within the field systems investigated. The iron extraction tests resulted in only ferrous iron, with non-detect levels of ferric iron, which should have been present if significant green rust phases were extracted during the test. In addition, the PHREEQC modeling predicted undersaturation of these phases within all of the waters. In general, the conditions appear to be too reducing to favor the formation of a mixed ($\text{Fe}^{+3}/\text{Fe}^{+2}$) phase such as green rust.

Magnetite and ilmenite were present in all of the samples but were not correlated with system performance. Evidence of dissolution of both minerals was common in all of the samples, suggesting that these phases may provide an important source of ferrous iron for iron sulfide precipitation when conditions are favorable (i.e., high rates of sulfate reduction).

As the iron sulfide phases have been shown to have relatively rapid reaction rates with chlorinated ethenes and iron sulfides are present within all of the samples (according to the AVS/CrRS results), the focus of the rest of the discussion is on the reactions that affect the rate of chlorinated ethene degradation by iron sulfide phases. An important conclusion of this study is that iron disulfides such as pyrite are more reactive than commonly thought and may be as reactive as iron monosulfides. A key factor affecting the reactivity of different iron sulfides is the surface area as described below.

4.1.2 Iron Sulfide Surface Area

The reaction between chlorinated ethenes and iron sulfide phases is believed to occur by the adsorption of the chlorinated ethene onto a finite number of reactive sites on the surfaces of the mineral, followed by reductive dechlorination and deactivation of the site (Lee and Batchelor, 2002a). Most investigators have assumed that the concentration of reactive sites on the mineral surfaces far exceeds the concentration of chlorinated ethene in solution such that a pseudo first order rate equation would apply. When TCE is the chlorinated ethene and FeS is the mineral, the rate equation is as follows:

$$-d[\text{TCE}]/dt = k[\text{FeS}][\text{TCE}] = k'[\text{TCE}] \quad (4-1)$$

Where,

$-d[TCE]/dt$	=	the rate of change in the concentration of TCE with time
k	=	the second-order rate constant ($L\ m^{-2}\ h^{-1}$)
k'	=	the pseudo first-order rate constant (h^{-1})
$[TCE]$	=	the concentration of TCE (M)
$[FeS]$	=	the concentration of reactive surface sites which is assumed to be proportional to surface area [$m^2\ L^{-1}$]

The reactive sites on the FeS are assumed to be proportional to iron sulfide surface area and constant in order to create a pseudo first order rate constant from a second order equation. However, by lumping $[FeS]$ into the rate constant (to create k') it makes the “constant” surface area dependant, such that rate constants for a given mineral can vary by orders of magnitude depending on the grain size of the particles and the total amount present. **Table 4-2** presents a summary of the specific surface areas (i.e., surface area per mass of material) for various grain diameters and phases (see Appendix E for calculations).

Table 4-2 - Relationship Between Particle Diameter and Calculated Geometric Specific Surface Area ^a

Median Grain Diameter (μm)	Mineral	Formula	Density (g/cm^3) ^c	Specific Surface Area (m^2/g)	Notes
0.004	Mackinawite	FeS_{1-x}	4.17	360	4 nm "nanoparticles"
0.004	Pyrite	FeS_2	5.03	298	4 nm "nanoparticles"
0.7	Pyrite	FeS_2	5.03	1.7	Approximate size of framboid microcrystals in OU-1 and the USEPA column samples
1	Pyrite	FeS_2	5.03	1.2	Median for the granular OU-1 samples
1	Mackinawite	FeS_{1-x}	4.17	1.4	Median for the granular OU-1 samples
8	Pyrite	FeS_2	5.03	0.149	Median for the Dover AFB samples
63	Pyrite	FeS_2	5.03	0.019	Minimum grain size of the pyrite used by Lee and Batchelor (2002a)
250	Pyrite	FeS_2	5.03	0.005	Maximum grain size of the pyrite used by Lee and Batchelor (2002a)

Table 4-2 - Relationship Between Particle Diameter and Calculated Geometric Specific Surface Area ^a (cont.)

Median Grain Diameter (μm)	Mineral	Formula	Density (g/cm ³) ^c	Specific Surface Area (m ² /g)	Notes
63 to 250	Pyrite	FeS ₂	5.03	27.8 ^b	Range of grain sizes of the pyrite used by Lee and Batchelor (2002a)
200	Pyrite	FeS ₂	5.03	0.042	10 μm thick coating on another grain (as observed for the USEPA column samples)

Notes:

a) Assumes cubic geometry

b) Surface area measured by the ethylene glycol monoethyl ether (EGME) method.

c) Density from Klein and Hurlbut, 1985.

The calculations were performed by assuming a cubic geometry. In addition, the surface areas assume smooth mineral surfaces and do not consider the rough surfaces exhibited by minerals such as pyrite which is evident in many scanning electron microscopy photographs. The surface area measured using the ethylene glycol monoethyl ether (EGME) method by Lee and Batchelor (2002a) for 63 to 250 μm particles of pyrite was 27.8 m²/g (reported in supporting information of Lee and Batchelor, 2002a). Assuming the smallest diameter in the range (63 μm) results in a “geometric” specific surface area of only 0.02 m²/g, which is three orders of magnitude lower. While the roughness correction is probably significant, three orders of magnitude difference suggests a laboratory error for the EGME measurement. Pugh et al. (1981) measured the specific surface area of 60 to 150 μm framboidal pyrite with 1 to 5 μm microcrystals at 2.0 m²/g using the Brunauer Emmett Teller method. Wolfe et al. (2007) obtained a specific surface area of 0.2 to 3.1 m²/g for ground and dry sieved pyrite with a grain size of 63 to 75 μm. The range reported by Wolfe et al. (2007) is only one to two orders of magnitude greater than the geometric surface area presented above. Therefore, it seems that the surface area obtained by Lee and Batchelor (2002a) is over-reported by one to two orders of magnitude. The over-predicted surface area affects the surface area-normalized rate constants that they provide (See **Table 3-35**) and likely the relative rates for the reduced iron minerals presented above.

In order to determine how the grain size for the field sites affects the abiotic rate constants a rough comparison was made between the calculated surface area and rate constants for the field sites and those in the literature. This approach was evaluated because the even though the total concentrations of iron sulfides (as measured by AVS and/or CrRS) at the Dover AFB site were equal to or greater than those at the Altus AFB site, the TCE degradation rate constants were significantly lower at the Dover AFB site. The difference in particle sizes provides one possible explanation for this difference.

First, the geometric specific surface area values shown in **Table 4-2** above were used along with the mulch physical properties (bulk density and total porosity) and the AVS/CrRS data to obtain

the total surface area (see Appendix E for calculation brief). Then, a single second-order rate constant (k) was calculated for AVS and CrRS iron sulfides. For the purpose of this example calculation, the reactivity of AVS and CrRS minerals were assumed to be equal for equal particle sizes. This assumption is reasonable based upon the earlier discussion in this section and in Section 4.1.1. Butler and Hayes (2001) obtained a first order abiotic rate constant (k') of $5.0 \times 10^{-4} \text{ h}^{-1}$ for a total of $0.5 \text{ m}^2 \text{ L}^{-1}$ FeS surface area for their experiment conducted at pH 7.3. These data were used to calculate a second order rate constant (k) of $0.001 \text{ L m}^{-2} \text{ h}^{-1}$. This second order rate constant was used to evaluate the site data as described below.

The total iron sulfide surface area was calculated from the specific surface area (see **Table 4-2**), the AVS and CrRS values, the bulk density, and the porosity (see the calculation brief in Appendix E). This approach may have underestimated the total surface area because of the limitations of the electron microprobe at resolving particle sizes on the nanoparticle scale. The total surface area for the OU-1 site (assuming one- μm particle diameters) was $7.2 \text{ m}^2 \text{ L}^{-1}$ of FeS and FeS₂. Therefore, assuming that FeS₂ has similar reactivity to FeS, the calculated pseudo first-order rate constant (k') for OU-1 was calculated to be $7.2 \times 10^{-3} \text{ h}^{-1}$, which is about a fourth of the measured value of $2.6 \times 10^{-2} \text{ h}^{-1}$ (**Table 4-3**). These values are considered reasonably close considering the various uncertainties and assumptions.

Table 4-3 - Overall and Surface Area-Determined Rate Constants for the Degradation of TCE

Site	Specific Surface Area (m^2/g)	Total FeS ₂ Surface Area (m^2/L) ^d	Total FeS Surface Area (m^2/L) ^e	Calculated Rate Constant k' (h^{-1}) ^a	Measured Rate Constant k' (h^{-1}) ^b
Altus AFB OU-1	2	5.41	5.61	1.10×10^{-2}	2.60×10^{-2}
	1.2/1.4 ^h	3.24	3.93	7.17×10^{-3}	
	2	7.66 ^j	11.5 ⁱ	1.91×10^{-2}	
Altus AFB SS-17	2 ^e	0	5.03	5.03×10^{-3}	3.29×10^{-1} to 3.42×10^{-3}
USEPA Column (Altus AFB SS-17) ^g	2	20	28	4.80×10^{-2}	1.19×10^{-2}
	0.49 ^f	4.97	6.96	1.19×10^{-2}	
Dover AFB – North Transect	0.2	0.54	1.60	2.13×10^{-3}	NA
Dover AFB – South Transect	0.2	3.59	5.12	8.71×10^{-3}	NA
Seneca Army Depot Activity – Wall A	2	4.47	2.32	6.79×10^{-3}	5.15×10^{-3} to 1.25×10^{-3}

Table 4-3 - Overall and Surface Area-Determined Rate Constants for the Degradation of TCE (cont.)

Site	Specific Surface Area (m ² /g)	Total FeS ₂ Surface Area (m ² /L) ^d	Total FeS Surface Area (m ² /L) ^c	Calculated Rate Constant k' (h ⁻¹) ^a	Measured Rate Constant k' (h ⁻¹) ^b
Seneca Army Depot Activity – Wall B	2	4.59	0.74	5.34 x 10 ⁻³	NA
Dugway Proving Ground	2	0.11	0.29	4.00 x 10 ⁻⁴	NA

Notes:

- a) Rate Constant k_{SA} (hr⁻¹) is the rate constant determined from the iron sulfide surface area of the biowall mulch and the abiotic rate constant determined by Butler and Hayes (2001) for FeS at pH 7.3.
- b) Rate constant based on TCE decrease between the UG and biowall locations as presented in **Table 3-35**.
- c) Calculated using the median AVS values, total porosity (0.25), bulk density (1.65 g/cc), and SSA.
- d) Calculated using the median CrRS values, total porosity (0.25), bulk density (1.65 g/cc), and SSA.
- e) Pugh et al. (1981).
- f) Adjusted to obtain value of k_{overall}.
- g) Using total porosity of 0.42 as reported in Shen and Wilson (2007) for the columns.
- h) Geometric surface area for 1 μm diameter cubes (pyrite/mackinawite), as reported in **Table 4-2**.
- i) Calculated using maximum AVS values, total porosity (0.25), bulk density (1.65 g/cc), and SSA.
- j) Calculated using maximum CrRS values, total porosity (0.25), bulk density (1.65 g/cc), and SSA.

Given that the roughness of the grains has not been taken into account, the total surface area could easily be double the geometric specific surface area. White and Peterson (1990) compared geometric surface areas to measured values for a wide range of minerals and obtained a roughness factor of seven times. Using the Brunauer-Emmett-Teller measured surface area obtained for framboidal pyrite (Pugh et al., 1981) results in a total surface area of 11.0 m²/L and a rate constant of 1.1 x 10⁻² h⁻¹. Using the maximum AVS and CrRS values (as opposed to the median) results in a total surface area of 19.1 m²/g and a pseudo first-order rate constant (k') of 1.91 x 10⁻² h⁻¹.

Iron sulfides were not identified in the Altus AFB SS-17 site samples during the electron microprobe analysis, so the grain size is unknown. However, using the grain size of the USEPA column samples (~1 μm) with the specific surface area determined by Pugh et al. (1981) and the median AVS value results in a total surface area of 5.03 m²/L and a pseudo first-order rate constant (k') of 5.03 x 10⁻³ h⁻¹, which is within the range of the measured k (3.42 x 10⁻³ to 3.29 x 10⁻¹ h⁻¹).

The Dover AFB rate constants were determined by assuming a specific surface area one-tenth that of the Altus AFB sites (0.2 m²/g) due to the larger grain size of the iron sulfides. The

calculated rate constants ($2.13 \times 10^{-3} \text{ h}^{-1}$ for N-Transect and $8.71 \times 10^{-3} \text{ h}^{-1}$ for the S-Transect) are comparable to the Altus AFB sites. The fact that similar effectiveness to the Altus AFB sites was not observed at Dover AFB suggests that the aged and oxidized nature of the iron sulfides at Dover AFB has had a significant negative effect on the second-order rate constant (k) that cannot be accounted for by grain size alone. The low pH of the Dover AFB groundwater compared to Altus AFB may also play a role, as is discussed in the next section.

A similar calculation for Seneca Army Depot Activity biowall A (assuming one- μm particles) resulted in a total surface area of $6.79 \text{ m}^2/\text{L}$ and a pseudo first-order rate constant (k') of $6.79 \times 10^{-3} \text{ h}^{-1}$, which is only slightly higher than the measured k' range of 1.3×10^{-3} to $5.2 \times 10^{-3} \text{ h}^{-1}$. The iron sulfide particle size for Seneca Army Depot Activity may be larger than the one- μm grains assumed in the calculations. Again, mackinawite nanoparticles do not appear to be present. The results for Biowall B were very similar ($5.34 \times 10^{-3} \text{ h}^{-1}$) to Biowall A.

The rate constant calculated for Dugway Proving Ground is an order of magnitude lower than for any of the other sites ($4.0 \times 10^{-4} \text{ h}^{-1}$) due to the low AVS and CrRS contents. The particle size was assumed to be one μm in the calculations, so a larger iron sulfide grain size at the Dugway Proving Ground would result in an even lower rate constant. The very low rate constant explains the negligible TCE removal within the reaction zone.

4.1.3 E_h /pH Conditions

The reaction rate constant for the abiotic dechlorination of TCE has been found to be pH-dependant for pyrite (Weerasooriya and Dharmasena, 2001) and mackinawite (Butler and Hayes, 2001). Weerasooriya and Dharmasena (2001) found that for pH values less than 6 the effect of pH was minor, but above pH 6 the rate constant for TCE reductive dechlorination increased dramatically. Butler and Hayes (2001) found a similar trend for TCE dechlorination by mackinawite. Data from Butler and Hayes (2001) was plotted and an exponential curve was fitted to the data using least-squares regression (see **Figure 4-1**).

An exponential curve was used because this allowed the rate to flatten out with decreasing pH, as was observed for pyrite by Weerasooriya and Dharmasena (2001) and does not result in a rate constant of zero (or a negative rate constant) for pH values less than about 7, which would happen if a linear trend was used.

The rate constants calculated using the empirical equation derived from **Figure 4-1** for the range of pH values observed for the field sites is presented in **Table 4-4**.

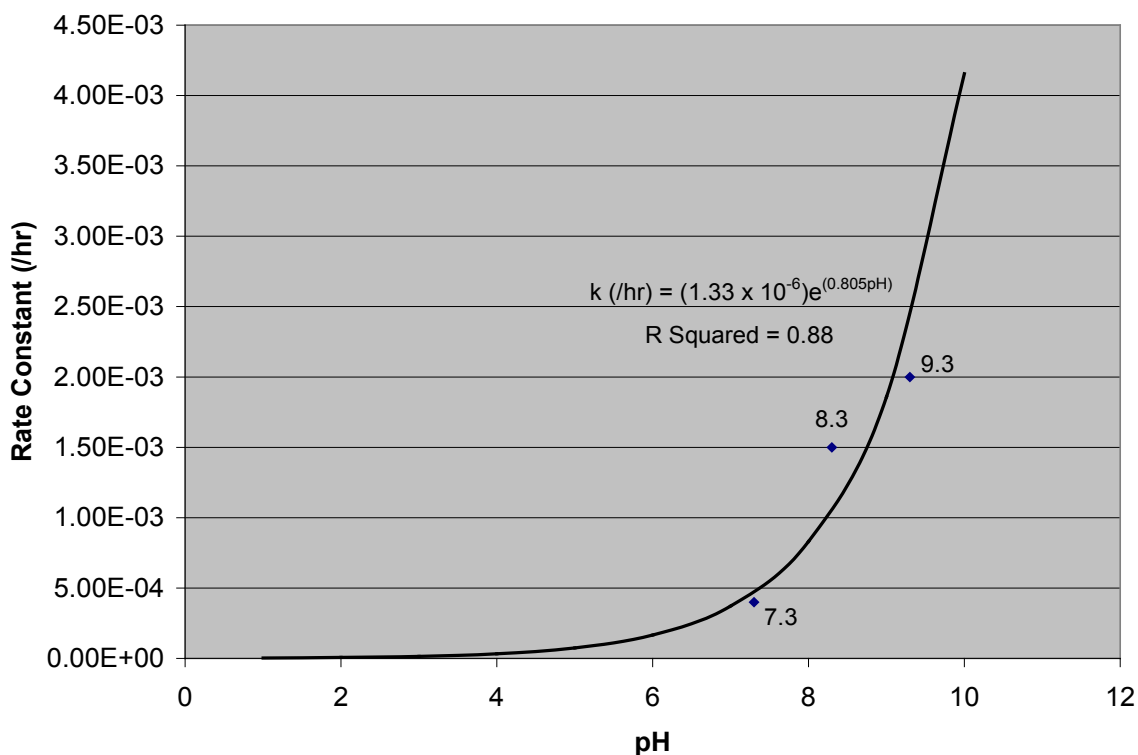


Figure 4-1 – Literature Data (Butler and Hayes, 2001) Documenting the Relationship Between Abiotic Reaction Rate and pH.

Table 4-4 - Dependence of the Rate Constant on pH ^a

pH	Rate Constant (h ⁻¹)	Notes
6	1.66 x 10 ⁻⁴	
7	3.72 x 10 ⁻⁴	2.2 times faster than at pH 6
8	8.31 x 10 ⁻⁴	5.0 times faster than at pH 6

Note:

a) Based on data from Butler and Hayes (2001).

The rate constants do not apply directly to the field sites, as the total surface areas are very different, but the relative effect of pH is the important factor. At the pH of the Dover AFB biowalls the pH is within the flat portion of the curve, but as the pH increases to the values consistent with the Altus AFB or Seneca Army Depot Activity sites the rate doubles, and as the pH reaches eight, the rate constant is five times greater.

Butler and Hayes (2001) also found that at increasing pH chloroelimination reactions (conversion to acetylene) was favored over dechlorination reactions (TCE → *cis*-1,2-DCE → VC, etc.).

In addition to affecting the reaction rate between chlorinated ethenes and the iron sulfides, pH also has an effect on the mineralogy of the iron sulfides. At lower pH values, the fraction of H₂S is greater relative to bisulfide than at higher pH, which could result in the conversion of iron monosulfide to iron disulfide by the rapid reaction proposed by Rickard (1997), consuming electrons in the process. Ideally, the electrons should be consumed during the reductive dechlorination of chlorinated ethenes rather than the reduction of hydrogen ions to hydrogen gas. Iron monosulfides are also less stable at lower pH values (Anderko and Shuler, 1997) and will not form if the pH is too low.

The E_h conditions must be low enough to produce enough dissolved sulfide and ferrous iron to reach saturation with respect to mackinawite. Simply reaching the stability field of pyrite is not adequate, as pyrite does not precipitate directly from solution, but must form via FeS precipitation through a series of alteration reactions (as previously discussed).

An E_h-pH plot for each of the sites is presented in **Figure 4-2**.

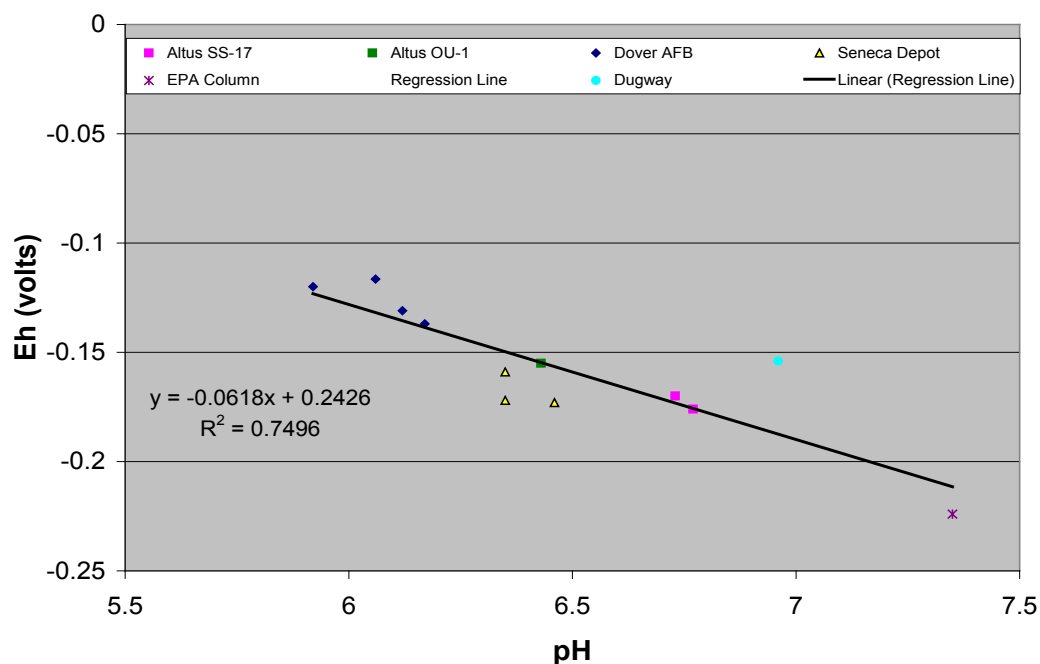
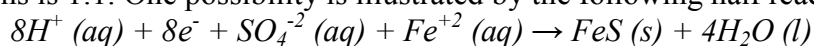


Figure 4-2 E_h-pH Relationship for Each Site

Figure 4-2 shows the relationship between E_h and pH for the reaction zone samples for each site. The slope of the least squares regression line is -1.04 in terms of pe (pe is $-\log[e^-]$), suggesting that the redox of the system is controlled by a reaction in which the ratio of protons (H⁺) to electrons is 1:1. One possibility is illustrated by the following half reaction:



The figure also shows that decreasing the E_h alone results in an increase in the pH (as would be expected).

4.1.4 Volumetric Sulfate Loading Rate

Sulfate availability has long been recognized as an important component in determining the rate of sulfate reduction in a system. Experimentation on passive treatment systems illustrated the usefulness of adding gypsum to the organic substrate (equivalent to the mulch in a biowall) to increase sulfide production and the rate of metal removal as sulfides (Whiting, 1994). The better performance of the Dover AFB-South Transect, where gypsum was added, compared to the North-Transect illustrates the importance of sulfate availability.

The reason that sulfide production rate is so important, is that the rate of production of FeS must be at least as great as the combined rates of chlorinated ethene dechlorination and reactive iron sulfide transformation to unreactive iron sulfides. Otherwise, the rate of production of iron sulfides becomes the rate-limiting step and the existing sulfides slowly convert to less reactive phases such as larger diameter more crystalline forms or other less reactive minerals such as greigite.

However, provision of sulfate alone is insufficient to promote high rates of reactive mineral formation and *in situ* biogeochemical transformation. Because reactive iron sulfides must continuously be generated in a heterogeneous system that is dependent on reactive solid surfaces (e.g., iron minerals and iron sulfide minerals), a dynamic system is required in which hydraulics and sulfate concentrations both play important roles. Groundwater flow through the treatment system is necessary to prevent generation of static geochemical conditions where reactive iron sulfides either are not produced or are converted to unreactive minerals. Sulfate must not become limiting else the potential for reactive iron sulfide formation diminishes.

The volumetric sulfate loading rate is a new term that considers both the contributions of sulfate concentration and system hydraulics. The volumetric sulfate loading rate is defined as the mass of sulfate flowing into the reactive system per unit volume of the reactive system per unit of time and is calculated using the following equation:

$$L_{SO_4} = C_{SO_4}(Q/V)$$

where,

L_{SO_4} = The volumetric sulfate loading rate to the biowall or bioreactor [mg L⁻¹ d⁻¹]

C_{SO_4} = The influent sulfate concentration [mg/L]

Q = The groundwater flow rate into the biowall or bioreactor [L/d]

V = The effective pore volume of the biowall or bioreactor [-]

The term Q/V is equal to the reciprocal of the hydraulic residence time of groundwater in the bioreactor or biowall. Thus the above equation can be written simply as:

$$L_{SO_4} = C_{SO_4}/\zeta$$

where,

ζ = The hydraulic residence time of groundwater in the biowall or bioreactor [d].

Table 4-5 presents calculated volumetric sulfate loading rates for the study sites. First order total VOC (i.e., sum of TCE, *cis*-1,2-DCE, and VC) degradation rate constants were the greatest at the Altus AFB sites and in the USEPA column. The volumetric sulfate loading rates were similarly greatest under these conditions. VOC degradation rates were significantly lower in cases where the volumetric sulfate loading rate was low. Dover AFB is particularly interesting because biowall samples had negligible abiotic VOC degradation while having high concentrations of AVS and CrRS. Electron microprobe analysis demonstrated that the iron sulfides were generally oxidized. The volumetric sulfate loading rate was low at this site because of a low groundwater velocity which did not promote a sufficiently dynamic system for reactive iron sulfide production.

Table 4-5 – Volumetric Sulfate Loading Rates

Site	First Order VOC Rate Constant (h ⁻¹)	Median AVS (mg-S/kg)	Median CrRS (mg-S/kg) ^a	Volumetric Sulfate Loading (mg L ⁻¹ d ⁻¹)
Altus AFB OU-1	6.3 x 10 ⁻³	174	23	167
Altus AFB SS-17 West Transect	1.1 x 10 ⁻²	226	285	65
Altus AFB SS-17 East Transect	6.3 x 10 ⁻³			
USEPA Column	1.0 x 10 ⁻²	1,450	1,518	98
Dover AFB North Transect - DG Biowall	0 ^b	441	218	0.082
Dover AFB South Transect - DG Biowall	0 ^b	1,414	1,453	1.7 ^c
Dover AFB North Transect - UG Biowall	0 ^b	441	218	0.082
Dover AFB South Transect - UG Biowall	0 ^b	1,414	1,453	1.7 ^c
Seneca Army Depot Activity Wall A	0 ^b	64	181	4.6
Seneca Army Depot Activity Wall B1	4.3 x 10 ⁻⁴	21	186	24
Seneca Army Depot Activity Wall B2	4.4 x 10 ⁻³			0.24
Dugway Proving Ground	0 ^b	80	43	NA

Note:

a) EAVS fraction not included.

b) Effluent concentrations were greater than influent concentrations so the rate constant was set to zero.

c) Does not account for sulfate loading from gypsum dissolution.

NA – Not applicable

4.1.5 Ionic Strength

The ionic strength of the solution (proportional to the salinity) is important in systems where nanoparticles are in suspension, because an increase in ionic strength results in coagulation of the particles and a decrease in the surface area and reactivity of the material. Vikesland et al. (2007) found that the reaction rate of nanoparticulate magnetite with carbon tetrachloride was a function of ionic strength, which the authors attributed to coagulation at high ionic strength (1 M). An evaluation of each of the sites shows that the ionic strength at Altus AFB (~0.1 M) and Dugway Proving Ground (~1 M) is too high to result in formation of nanoparticles of mackinawite. However, Dover AFB and Seneca Army Depot Activity have low enough ionic strengths (0.01-0.04 M) where nanoparticles could be present. However, in addition to low ionic strength, a fast nucleation rate (compared to crystal growth rate) is required. Fast nucleation of iron sulfides occurs when the solution is supersaturated (Butler and Rickard, 2000). Supersaturation can result when the rate of sulfate and iron reduction are faster than the rate of iron sulfide precipitation. At low ionic strength, and when the iron and sulfate reduction processes are optimized, nanoparticle production may be possible. Ohfuji and Rickard (2006) measured specific surface areas of 186 to 579 m²/g for nanoparticulate mackinawite, which are two orders of magnitude greater than for 1 µm particles. Optimizing conditions for the production of mackinawite nanoparticles could dramatically increase the chlorinated ethene dechlorination rate to values potentially greater than for the Altus AFB sites.

None of the sites investigated exhibited evidence of nanoparticulate formation (i.e., apparent supersaturation with respect to mackinawite or very high abiotic degradation constants). Thus the importance of ionic strength with respect to *in situ* biogeochemical transformation requires further study.

4.1.6 Organic Carbon

Organic carbon is important in that a minimum amount is required to drive biological sulfate reduction and other bacterial processes. Clearly 0.08 percent organic carbon in the solid samples was not enough, as illustrated by the Dugway site, but 2.8 percent was sufficient, as illustrated by the Altus AFB SS-17 site. The SS-17 mulch also had a low lignin content (4.7 percent for the tree mulch) making the organic carbon easier for the bacteria to break down into monomers.

The dissolved organic carbon or total organic carbon in the groundwater tended to be lower for the systems in which abiotic transformation was dominant (Altus AFB sites) than for systems where biotic reactions predominate (Dover AFB). However, sulfate-reducing bacteria are not the only bacteria that use organic carbon. Seneca Army Depot Activity wall A has a low organic carbon content within the wall, but the methanogenic activity is very high, suggesting that the methanogens rather than the sulfate-reducing bacteria are consuming the dissolved organic carbon. The high groundwater total organic carbon at Dover AFB suggests that the organic matter is being broken down at a sufficient rate. However, without knowing the composition of the total organic carbon in terms of the amount of organic acids and alcohols it is not possible to determine if the fermenters have converted the monomers into forms that can be used by the sulfate-reducing bacteria. Volatile fatty acid data for the sites suggest that acetic acid concentrations are initially high but decrease below detection levels once dissolved organic carbon concentration decreases to less than 50 to 80 mg/L.

4.1.7 Dissolved Oxygen

Sulfate-reducing bacteria operate under anaerobic conditions, so low dissolved oxygen concentrations are essential to optimum performance. In addition, dissolved oxygen can react with iron sulfide phases to form an unreactive iron sulfate surface coating on the grains. Reactions may still proceed, but the rate is much slower as electrons must diffuse through the sulfate layer in order to react with the chlorinated ethenes. The periodic influx of oxygenated precipitation into the biowalls at Dover AFB may explain the high oxygen content of the sulfide grains determined by the electron microprobe analysis (~10 percent oxygen). The mounding observed in monitoring wells following precipitation events is evidence that significant rainwater enters the biowall. Thus placement of impermeable caps on biowalls and bioreactors to limit infiltration is recommended.

4.1.8 Iron Oxide Mineral Surface Area

The USEPA column samples illustrate that iron oxide minerals such as magnetite and hematite can provide surface sites for the formation of iron sulfides. Therefore, the addition of iron oxides to the mulch should have a beneficial effect. The higher rate constant range for the BB04 transect in which magnetite was added to the mulch mix than for transect BB05 in which magnetite was not added may be due to coating of magnetite grains with iron sulfides. However, the iron sulfides that are added by coating sand-sized grains have low specific surface area compared to precipitation of frambooids or micron-sized grains. Iron ores (e.g., magnetite and hematite) should be finely crushed prior to use to increase surface area.

4.2 Summary of Field System Performance

A summary of the variables and performance for each site is presented in **Tables 4-6** through **4-8**. The following sections will discuss the performance of each site using the criteria presented in Section 4.1 and the results presented in **Tables 4-6** through **4-8**. The parameters discussed below include only those that were found to be useful or that were important in distinguishing the best performing systems.

Table 4-6 - Summary of Soil Results for Each Site

Analysis	Altus AFB SS-17	USEPA Column	Altus AFB OU-1	Dover AFB North Transect	Dover AFB South Transect	Seneca Army Depot Activity	Dugway Proving Ground
Iron Phases Present (EMP)	Crystalline magnetite	FeS ₂ associated with crystalline magnetite and hematite	FeS ₂ , crystalline magnetite	Partially to completely oxidized FeS and FeS ₂	Partially to completely oxidized FeS and FeS ₂	Crystalline and amorphous magnetite	Ti-bearing hematite or ferrous hydroxide, and ilmenite (some reacted)
Iron Phases Present (AVS/CrRS)	AVS (174 mg-S/kg) ^a and CrRS (23 mg-S/kg) ^b	AVS (1450 mg-S/kg) ^a and CrRS (1518 mg-S/kg) ^b	AVS (226 mg-S/kg) ^a and CrRS (285 mg-S/kg) ^b	AVS (441 mg-S/kg) ^a and CrRS (218 mg-S/kg) ^a	AVS (1414 mg-S/kg) ^a and CrRS (1453 mg-S/kg) ^a	AVS (186 mg-S/kg) ^a and CrRS (21 mg-S/kg) ^a	AVS (80 mg-S/kg) ^a and CrRS (43 mg-S/kg) ^a
Iron Phases at Saturation (PHREEQC)	Troilite (FeS)	Poorly ordered Mackinawite (FeS)	Troilite (FeS) and mackinawite (FeS)	Troilite (FeS), poorly ordered mackinawite (FeS), and crystalline mackinawite (FeS)	Troilite (FeS), amorphous FeS, and mackinawite (FeS)	Greigite (Fe ₃ S ₄), poorly ordered mackinawite (FeS), and alkaline mackinawite (FeS)	Poorly ordered mackinawite (FeS), and mackinawite (FeS)
Median Organic Carbon Content (%)	2.80%	4.20%	9.10%	4.3% (UG wall), 4.6% (DG wall)		6.0% (wall A), 7.9% (wall B)	0.08%

Notes:

a) Median AVS result.

b) Median CrRS not including AVS fraction.

Table 4-7 - Summary of Water Analyses and Modeling Results for Each Site

Analysis	Altus AFB SS-17	USEPA Column	Altus AFB OU-1	Dover AFB North Transect	Dover AFB South Transect	Seneca Army Depot Activity	Dugway Proving Ground
Total or Dissolved Organic Carbon in Reaction Zone (mg/L)	10.6 ^c (BB04W) 10.4 ^c (BB05W)	5.39 ^d	18.2 ^d (MP1)	16 ^d (TS-MW01) 33 ^d (TS-MW03)	2.8 ^d (TS-MW06) 63 ^d (TS-MW08)	13 ^d (TEMP-1) 167 ^d (MWT-27) 92 ^d (MWT-28)	121 ^c (TW-28)
H ₂ S Concentration (mol/L) (PHREEQC)	7.24 x 10 ⁻⁰⁶ (BB04W) 6.33 x 10 ⁻⁰⁶ (BB05W)	5.90 x 10 ⁻⁰⁵ (column B3)	9.12 x 10 ⁻⁰⁶ (MP1)	3.76 x 10 ⁻⁰⁵ (TS-MW01) 4.35 x 10 ⁻⁰⁵ (TS-MW03)	8.92 x 10 ⁻⁰⁵ (TS-MW06) 1.40 x 10 ⁻⁰³ (TS-MW08)	3.57 x 10 ⁻⁰⁵ (TEMP-1) 7.92 x 10 ⁻⁰⁶ (MWT-27) 3.03 x 10 ⁻⁰⁵ (MWT-28)	2.42 x 10 ⁻⁰⁵ (TW-28)
Sulfate/Sulfide E _h in Reaction Zone (PHREEQC)	-176 (BB04W) -170 (BB05W)	-224 (column B3)	-155 (MP1)	-120 (TS-MW01) -137 (TS-MW03)	-117 (TS-MW06) -131 (TS-MW08)	-159 (TEMP-1) -173 (MWT-27) -172 (MWT-28)	-128 (TW-28)
Dissolved Oxygen in Reaction Zone (mg/L)	0.05 (BB04W) 0.05 (BB05W)	4.11 (column B3)	0.05 (MP1)	0.59 (TS-MW01) 0.36 (TS-MW03)	0.57 (TS-MW06) NA (TS-MW08)	0.30 (TEMP-1) 0.33 (MWT-27) 0.49 (MWT-28)	0.85 (TW-28)
pH in Reaction Zone	6.77 (BB04W) 6.73 (BB05W)	7.35 (column B3)	6.43 (MP1)	5.92 (TS-MW01) 6.17 (TS-MW03)	6.06 (TS-MW06) 6.12 (TS-MW08)	6.35 (TEMP-1) 6.46 (MWT-27) 6.35 (MWT-28)	6.30 (TW-28)
Ionic Strength (M)	0.083 (BB04W) 0.091 (BB05W)	0.084 (column B3)	0.053 (MP1)	0.008 (TS-MW01) 0.014 (TS-MW03)	0.021 (TS-MW06) 0.038 (TS-MW08)	0.017 (TEMP-1) 0.034 (MWT-27) 0.029 (MWT-28)	0.967 (TW-28)
Iron Concentration in up gradient Groundwater (mg/L)	0.20 (BB04U) 0.10 (BB05U)	0.00 (column B3)	<0.027 (EPAUMP1)	1.0 (TS-MW11) 1.9 (TS-MW03)	0.01 (TS-MW12) 1.32 (TS-MW07)	0.06 (MWT-25) 0.04 (MWT-26) 66 (MWT-27)	0.09 (MWT-25)

Table 4-7 - Summary of Water Analyses and Modeling Results for Each Site (cont.)

Analysis	Altus AFB SS-17	USEPA Column	Altus AFB OU-1	Dover AFB North Transect	Dover AFB South Transect	Seneca Army Depot Activity	Dugway Proving Ground
Major Ion Chemistry of Groundwater	~Equal mix of all	~Equal mix of all	Ca(HCO ₃ /SO ₄)	CaHCO ₃	CaHCO ₃ (CaSO ₄ where gypsum was added)	CaHCO ₃	NaCl
Sulfate Concentration in up gradient Groundwater (mg/L)	1,780 (BB04U) 1,560 (BB05U)	1,670 (column B3)	1,890 (EPAUMP1)	6.4 (TS-MW11) 15 (TS-MW03)	34 (TS-MW12) 970 (TS-MW07)	Wall A 190 (MWT-25) Wall B1 1,000 ^b (MWT-26) Wall B2 10.0 (MWT-27)	12,400 (MWT-25)
Sulfate Sources/Sinks (PHREEQC)	CaSO ₄ phase ^a present in aquifer matrix	CaSO ₄ phase ^a present in aquifer matrix	CaSO ₄ phase ^a present in aquifer matrix	No sulfate present except in aquifer matrix	No sulfate present except where gypsum added	No sulfate present in aquifer matrix	CaSO ₄ phase ^a present in aquifer matrix
Calcite Precipitation in Wall (PHREEQC)	Calcite likely precipitating in wall and DG aquifer	Calcite likely precipitating in column	Calcite likely precipitating in wall and DG aquifer	None	Calcite likely precipitating in wall where gypsum was added	None	Calcite likely precipitating in wall and DG aquifer
Initial TCE or PCE Concentration (µg/L)	3,933 (BB04U) 154 (BB05U)	2,585 (column B3)	550 (EPA-UMP1)	5.1 PCE (TS-MW02) 11 PCE (TS-MW11)	2.4 PCE (TS-MW12) 11 PCE (TS-MW07)	26 (MWT-25) 2.8 (MWT-26) <10 (MWT-27)	1,900 (TW-25)

Notes:

- a) Gypsum or anhydrite.
- b) Likely in error based on charge and mass balance evaluation and previous analyses.
- c) Dissolved organic carbon.
- d) Total organic carbon.

Table 4-8 - Summary of System Design and Performance for Each Site

Analysis	Altus AFB SS-17	USEPA Column	Altus AFB OU-1	Dover AFB North Transect	Dover AFB South Transect	Seneca Army Depot Activity	Dugway Proving Ground
System Design							
Mulch Mix ^d	Tree mulch (42%), cotton gin trash (11%), concrete sand (32%), and gravel (15%). (magnetite added to B4 transect area).	Tree mulch (48% with 4.7% lignin content), cotton gin trash (10% with 9.6% lignin), river sand (38%), and hematite (4%).	Tree mulch (48%), cotton gin compost (10%), and river sand (42%).	Tree mulch (50%), silty river sand (45%), and limestone (5%).	Tree mulch (50%), silty river sand (40%), limestone (5%), and gypsum (5%).	Mulch (50%) and sand (50%). Mulch in UG biowall coated with vegetable oil.	Direct injection of emulsion of vegetable oil, lecithin, sodium bromide, and site groundwater.
Residence Time (days)	1-50	17	9-13.7	130 (UG wall), 195-391 (DG wall)	130 (UG wall), 195-391 (DG wall)	16-66	N/A
System Performance							
Percent Abiotic Transformation	99.85% (BB04 Transect). 97.84% (BB05 Transect).	49% to 88% ^a 98.50% (this study)	82.70%	VOC ^c concentrations increased in the wall relative to up gradient.	VOC ^c concentrations increased in the wall relative to up gradient.	VOC ^c concentrations increased in the wall relative to up gradient (Wall A), 50.43% (Wall B1), 98.79% (Wall B2).	TCE concentrations increased in the Injection Well relative to up gradient.
Plume Trend	Abiotic (parallel decline in VOCs).	NA	TCE abiotic. Biotic transformation of cis-DCE to VC (at least 82%).	VOCs increase.	VOC trends are largely flat (little or no transformation).	VOCs increased in wall A. VOC concentrations up gradient of wall B are too low to determine a trend.	TCE concentrations increased in the Injection Zone relative to up gradient.

Table 4-8 - Summary of System Design and Performance for Each Site (cont.)

Analysis	Altus AFB SS-17	USEPA Column	Altus AFB OU-1	Dover AFB North Transect	Dover AFB South Transect	Seneca Army Depot Activity	Dugway Proving Ground
Overall Transformation Rate (h ⁻¹)	3.3 x 10 ⁻¹ to 6.6 x 10 ⁻³ (BB04 Transect) 1.7 x 10 ⁻¹ to 3.4 x 10 ⁻³ (BB05 Transect)	1.2 x 10 ⁻²	1.2 x 10 ⁻²	PCE concentrations increased in the wall relative to up gradient.	PCE concentrations increased in the wall relative to up gradient.	1.3 x 10 ⁻³ to 5.2 x 10 ⁻³ (Wall A).	TCE concentrations increased in the Injection Zone relative to up gradient.
TCE or PCE Percent Removal ^b	98.35-99.96% of TCE	99.33% of TCE	99.98% of TCE	PCE and TCE concentrations increased in the wall relative to up gradient.	PCE and TCE concentrations increased in the wall relative to up gradient.	86.15% of TCE (Wall A) TCE DL of 10 µg/L in Wall B sample (MWT-27) was higher than the up gradient well concentration of 2.8 µg/L.	TCE concentrations increased in the Injection Zone relative to up gradient.

Notes:

a) Shen and Wilson, 2007.

b) Between upgradient well and in-wall well.

c) "VOCs" in this case included the sum of the molar concentrations of PCE+TCE+cis-DCE+VC+ethene+ethane.

d) All percentages by volume.

NA - not analyzed.

4.2.1 Altus AFB SS-17 and OU-1 Sites

The Altus AFB sites can be discussed together, because the performance of the two sites was very similar (rate constants were similar), they both were characterized by abiotic transformation, they received the same groundwater, and the mulch formulations were similar. The Altus AFB sites had the highest percent abiotic character, the highest abiotic and overall rate constants and the highest TCE removal rates of any of the sites. The conditions which resulted in effective TCE treatment included the following:

- The total surface area of the iron sulfides was high due to a high concentration of iron sulfides in the mulch and the high specific surface area of the 1 μm granular particles and framboid microcrystals.
- The pH of the Altus AFB sites and USEPA column (6.4-7.4) were among the highest of the sites (but not the highest), while the Eh was sufficiently low (-224 to -155 mV) for formation of iron monosulfides.
- The ionic strength of the groundwater (0.05 to 0.09 M) was too high to allow mackinawite nanoparticles to persist, otherwise, the rate constants may have been even greater.
- The concentrations of organic carbon in the biowall matrix (2.8 to 9.1 percent) were sufficient for the sulfate-reducing bacteria and the other critical reactions (i.e., fermentation to remove acetylene)
- The TCE concentrations were the highest of any of the sites (154 to 3,993 $\mu\text{g/L}$), especially SS-17 (3,993 $\mu\text{g/L}$).
- Dissolved oxygen was low (0.05 mg/L) with the exception of the column study (4.1 mg/L), and there appeared to be minimal infiltration of precipitation into the biowalls, which has minimized oxidation of the iron sulfides.
- The surface area of iron oxides is high, especially where the mulch has been amended with magnetite.

4.2.2 Dover AFB

The relatively poor performance of the Dover AFB biowalls was due to the following factors:

- The total iron sulfide content was similar to the Altus AFB sites (441 to 1,414 mg/kg for FeS and 218 to 1,453 mg/kg for FeS₂), but the median iron sulfide particle size was 8 μm compared to 1 μm for Altus AFB which decreased the specific surface area significantly. Therefore, the total surface area was similar. The larger particle size observed in the Dover samples likely resulted from an Ostwald Ripening process in which fine grained iron monosulfides dissolve while pyrite grains continue to grow. Such a process would occur when infiltration water enters the wall, resulting in dissolution of iron monosulfides but not the more stable pyrite phases.
- The pH was the lowest of all of the sites (5.9 to 6.2). The low pH alone for Dover AFB results in a 50 percent decrease in the rate constant compared to the Altus AFB sites. The E_h at Dover AFB was the highest of all of the sites, which is not optimal for sulfate-

reducing bacteria or for the production of reactive iron sulfides (i.e., iron monosulfides vs. greigite).

- The sulfate concentrations were very low in the north transect (6.4 to 15 mg/L) which further limited the sulfate reduction rate. In the south transect, where gypsum was added, the performance was improved, but was not optimal. The mass loading of sulfate was also low due to the very low groundwater velocity (reflected by the very long residence time).
- The ionic strength at Dover AFB (0.01 to 0.04 M) is low enough to prevent nanoparticle coagulation, but the sulfate and iron reduction rates are not fast enough to result in supersaturation of mackinawite and rapid nucleation.
- The organic carbon content (4.3 to 4.6 percent) was sufficient.
- The chlorinated ethene concentrations (2.4 to 11 $\mu\text{g/L}$ PCE), particularly in the downgradient walls were low, resulting in low reaction rates.
- Dissolved oxygen, while typically low (0.4 to 0.6 mg/L), is often high due to infiltration of precipitation following storm events. The dissolved oxygen oxidized the sulfides present in the mulch which produced a significant decrease in the rate of reaction with chlorinated ethenes.
- The presence or absence of iron oxides was only important in terms of providing a source of ferric iron for reduction to ferrous iron, because the rate of sulfide production does not appear to be rapid enough to coat iron oxide grains with iron sulfides.

4.2.3 Seneca Army Depot Activity

The moderate performance of the Seneca Army Depot Activity system can be explained by the following factors:

- The specific surface area of the sulfides is unknown, because no grains were identified during the electron microprobe analysis. However, the relatively low concentrations of sulfides in the mulch suggest that the total surface area is lower than for the Altus AFB sites (except for SS-17, which is based on a small and possibly unrepresentative number of samples). Based on the rate constant and the relationship between surface area and rate constant presented above (Section 4.1.2), the particle size for the Seneca Army Depot Activity site should be about 1 μm . The low production rate of iron sulfides has allowed the existing iron sulfide grains to age and oxidize to relatively unreactive greigite.
- The Eh-pH conditions for Seneca Army Depot Activity are comparable to Altus AFB and in some cases the pH is higher (6.4 to 6.5 in reaction zone) and the Eh is lower (-173 to -159 mV) than for Altus AFB. Therefore, the Eh-pH conditions appear to be favorable.
- Seneca Army Depot Activity has low sulfate concentrations in the up gradient groundwater (10 to 190 mg/L) and does not have a source of sulfate present within the aquifer or amended into the mulch mix. Therefore, the rates of sulfate reduction are low, despite the favorable E_h-pH conditions.

- The ionic strength is low enough where nanoparticles could persist (0.02 to 0.03 M), but the rate of sulfide production not fast enough to cause supersaturation and rapid nucleation of FeS.
- The organic carbon content (6 to 8 percent) is sufficient.
- The chlorinated ethene concentrations are relatively low (2.8 to 26 µg/L), especially in the downgradient biowalls (B1/B2).
- Dissolved oxygen concentrations are generally low (0.3 to 0.5 mg/L), but occasionally spike above 2 mg/L. The dissolved oxygen spikes may have resulted in the formation of iron sulfate coatings on the grains.
- The presence or absence of iron oxides was only important in terms of providing a source of ferric iron for reduction to ferrous iron, because the rate of sulfide production does not appear to be rapid enough to coat iron oxide grains with iron sulfides.

The relatively low performance of the Seneca Army Depot Activity biowalls is due to the low sulfate concentrations and thus a low sulfate loading to the biowalls. Total organic carbon is sufficient and the methanogenic bacteria are very active. Because of the low upgradient sulfate concentrations, moderate amounts of iron sulfides (AVS/CrRS results) have been produced but appear to have aged to relatively unreactive greigite (electron microprobe results).

4.2.4 Dugway Proving Ground

The Dugway vegetable oil injection system did not provide any significant treatment of chlorinated ethenes in the groundwater. The reasons for the lack of performance can be explained as follows:

- The iron sulfide grain size is unknown, because no grains were found during the electron microprobe analysis. However, the total iron sulfides present was very low, suggesting that the total surface area is also low.
- The Eh/pH conditions for Dugway Proving Ground are generally favorable (pH = 6.3 and Eh = -128 mV in the reaction zone), and the geochemical modeling indicated that FeS was at saturation within the groundwater.
- The sulfate supply at Dugway Proving Ground was more than sufficient for the sulfate-reducing bacteria. In fact, the sulfate concentrations may be too high. Hilton and Oleszkiewicz (1988) found that sulfate-reducing bacterial activity is inhibited (but not eliminated completely) by sulfate concentrations in excess of 1,200 mg/L.
- The ionic strength is too high (1 M) to allow nanoparticles to persist.
- The very low organic carbon content in the aquifer matrix of the injection zone at Dugway Proving Ground (0.08 percent) appears to be the most important deficiency of the system.
- The chlorinated ethene concentrations are high (1,900 µg/L TCE), such that if the sulfide production rate was higher, the initial reaction rate should be high.
- The dissolved oxygen concentrations have been consistently <1 mg/L, which should be ideal.

- Abundant iron oxide minerals, many showing evidence of dissolution were present. Therefore, production of ferrous iron does appear to be occurring. However, without sufficient sulfide production rates iron sulfides cannot be formed.

The lack of performance of the Dugway proving Ground vegetable oil injection system is likely related to the relatively low production rate of reactive iron sulfides precipitation, which can be traced back to low total organic carbon concentrations. The hydrogen sulfide odor observed by the field crew, the presence of “black staining” on the aquifer sediment, and the saturation with respect to mackinawite all indicate that some iron sulfide is being produced. However, the AVS/CrRS and electron microprobe results indicated that very little precipitation of the phase has occurred, at least at location TMW-28 within the injection zone. Because the abiotic TCE transformation rate is directly related to total surface area of iron sulfide, the low production rate of iron sulfide has resulted in very low to negligible TCE degradation rates.

4.3 Strategies for Maximizing System Performance

4.3.1 Maximizing Iron Sulfide Surface Area

The most important factor in maximizing the rate of reaction between chlorinated ethenes and iron sulfides is the surface area of the iron sulfides. While adjusting the pH from 6 to 8 can increase the rate constant by a factor of five (all other variables remaining constant), a decrease in the median grain size of the iron sulfide particles from 1 μm to 10 nm can increase the rate constant by 100 times. Although nanoparticles were not likely present in any of the field systems investigated in this study, several investigators have reported the production of nanoparticulate iron monosulfides by sulfate-reducing bacteria (Ohfuji and Rickard, 2006).

In general, to produce small diameter iron sulfide particles, the nucleation rate must be very rapid compared to the rate of crystal growth (Butler and Rickard, 2000). Such conditions are produced when the solution is supersaturated with respect to the iron sulfide mineral (Butler and Rickard, 2000). In order to get supersaturated conditions, the ferrous iron and sulfide must be added to the system very quickly, such as occurs in the laboratory when the two solutions are mixed together. Most laboratory preparation of nanoparticulate mackinawite involves the addition of a sulfide solution, such as sodium sulfide to a ferrous solution, such as ferrous chloride (Ohfuji and Rickard, 2006).

In a biowall, the production of sulfide and ferrous iron are controlled by the activity of sulfate-reducing bacteria and iron-reducing bacteria or abiotic iron reduction, respectively. In order to create ferrous iron and sulfide quickly, the conditions for the bacteria must be ideal, providing sufficient useable organic carbon, sulfate, and favorable E_h -pH conditions. In some respects, the system is self-limited in the amount of sulfide that can be generated, because too much sulfide can be toxic to sulfate-reducing and other bacteria (Gusek and Wildeman, 2002).

Postgate (1984) suggested a pH of greater than 5 and oxidation-reduction potential less than or equal to -100 mV are the minimum requirements for the sulfate-reducing bacteria to thrive. However, these are rather broad requirements and other factors need to be considered, such as the type of substrate used in the biowall.

Not all organic carbon has the same degree of bioavailability. Before sulfate-reducing bacteria can use the organic carbon from the mulch, the plant cell walls must first be broken down into bioavailable forms. Cell walls are composed of three main constituents, cellulose, hemicellulose, and lignin. Lignin is by far the most difficult part to biodegrade (Kirk and Farrel, 1987), requiring fungi and other organisms that operate under aerobic conditions. Because sulfate-reducing bacteria require anaerobic conditions, lignin tends to persist in these systems for long periods of time (Van Soest, 1994). Therefore, the bioavailability of the substrate is directly dependent upon the lignin content; the higher the lignin the lower the bioavailability. The lignin content of plant mulch varies greatly. For example, the tree mulch used for the Altus AFB SS-17 site had a lignin content of only 4.7 percent (Shen and Wilson, 2007) and was apparently quite effective. In general, hardwoods tend to have low lignin content while pines have high lignin (<http://compost.css.cornell.edu/lignin.table.html>). Some of the reported values include; beech tree 12.7 percent, sugar maple 8.49 percent, cow manure 7.9 to 10.1 percent, corn stalks 3.9 percent, pine 27.8 percent, and spruce 28.6 percent. Clearly, not all tree mulch is the same, and the bioavailability may be vastly different from one type to the next. Research into substrate mixtures for passive treatment systems for acid rock drainage is voluminous, and contains useful information on the best substrate formulations for optimizing sulfate reduction. Early passive systems used manure or mushroom compost mixed with hay, but the permeability of such systems tended to be low and the organic carbon tended to be short-term in nature (Whiting, 1994). More recent mixtures have used wood chips as a permeable and long-term form of organic carbon (Gusek, 1998), and even more recently corn stover and walnut shells have been used (Figueroa et al., 2007). Mulch composition has also been discussed specifically in the context of biowalls (AFCEE, 2008; Groundwater Services, Inc., 2005; Ahmad et al., 2007).

4.3.2 pH Adjustment/Buffering

Adjustment of the pH of the groundwater upgradient or in the biowall could be conducted to increasing the abiotic TCE degradation rate constant by five times or more. However, modifying the pH may be difficult depending on the buffering capacity of the aquifer sediments. Use of limestone can be a practical means of increasing or buffering pH. The use of buffers within the biowall, such as limestone can be effective unless the system is at saturation with respect to calcite. Soluble or liquid amendments can also be used. The addition of alkalinity may also have unintended and possibly negative effects, such as removal of dissolved ferrous iron in the form of the mineral siderite, which is slow to react with chlorinated organic compounds (Elsner et al. 2004).

The pH should not be increased too much (>9), because negative effects on the bacteriological systems and iron sulfide minerals may result.

4.3.3 Volumetric Sulfate Loading Rate

The hydraulic residence time in combination with the influent sulfate concentration determines the sulfate loading rate to the biowall. The sites with the highest sulfate loading rate and the shortest residence times (i.e., Altus AFB OU-1 and SS-17) were the most effective, while the sites with the lowest sulfate loading rate and the longest residence times were among the least effective (i.e., Seneca Army Depot Activity and Dover AFB). The low sulfate loading rate limited the formation of reactive iron sulfides and biogeochemical TCE transformation. The low sulfate loading rate results in a slow rate of production of iron sulfides, resulting in a coarse

precipitate with relatively low surface area. The low sulfide production rate also causes the iron sulfides that are present to age and recrystallize or to convert to less reactive forms such as greigite. Therefore, systems should be designed with the sulfate loading rate in mind.

For systems in which the natural sulfate concentrations are low (less than about 200 mg/L), sulfate could be added as a direct addition to the mulch mix (such as was done in the south transect at Dover AFB). Gypsum addition is particularly well suited to a site such as Seneca Army Depot Activity where the main deficiency of the system appears to be the sulfate supply. Soluble sources of sulfur can also be added especially in the case of recirculating bioreactors.

For systems where the groundwater velocity is low a recirculation bioreactor may be required in order to increase the dynamics of the system. In bioreactor systems, optimization of the sulfate concentration and groundwater flow rate may be necessary to determine the most cost-effective way to increase the volumetric sulfate loading rate.

Addition of other forms of sulfur to the mulch, such as pure sulfur could also be explored. Pure sulfur would have the advantage over gypsum of adding a more reduced form of sulfur to the system that could be utilized by sulfur-reducing bacteria. Sulfur would also be effective at removing oxygen and nitrate from the influent groundwater, helping to preserve the sulfide produced by the bacteria. However, the effectiveness of such a system is unknown. Nevertheless, denitrifying bacteria have been shown to use sulfur as an electron donor to convert nitrate to nitrogen gas (Zhang, 2002).

4.3.4 Organic Carbon Addition

Addition of dissolved organic carbon in the form of lactate, acetate, ethanol, or molasses is a proven technique for increasing the productivity of sulfate-reducing bacteria within passive treatment systems (Whiting, 1994; Kennedy et al., 2006; Buccambuso et al. 2007a, 2007b). Dissolved organic substrate could be injected into the aquifer upgradient of the biowall. While the operations and maintenance costs would increase with a requirement for periodic injections, a system which is currently not performing very well could be made to function as originally intended. Vegetable oil can also be added to existing biowalls and typically will last longer than soluble electron donors.

4.3.5 Other Strategies

Other strategies would include capping areas directly above and just upgradient of the biowalls to limit infiltration of oxygenated precipitation or to add iron oxide minerals to the mulch mix (such as was done at Altus AFB SS-17 Transect B4). Iron oxide addition to the mulch is easy to do, but the resulting iron sulfide is as a grain coating with very low specific surface area. The very modest improvement in the rate constant between the B4 and B5 transects at SS-17 is likely due to grain coating by iron sulfides (although none were found in the field samples, only the USEPA column samples). Increasing the supply of ferrous iron could also be helpful, either as an upgradient injection of a ferrous solution or addition of ferrous iron minerals to the mulch mix. The injection of ferrous iron solutions into an aquifer is problematic, as it is difficult to prevent oxidation of the iron and subsequent precipitation as iron oxyhydroxides. The iron mineral addition may be limited by adsorption of bisulfide (HS^-) ions onto the surface followed by coating of the grains with an iron sulfide mineral (Hanoch et al., 2006), limiting the dissolution

of the mineral. The adsorption of negatively charged bisulfide ions could be limited for minerals with a low pH of zero-point-of-charge (pH_{zpc}), such as hematite. Therefore, hematite is likely to be a much better source of iron than magnetite, as it is less likely to become coated with iron sulfide at $\text{pH} > 6.7$, as demonstrated by the USEPA column samples.

Another possible iron source is the ferrous iron carbonate mineral siderite (FeCO_3), which was undersaturated in the Altus AFB groundwaters but not for the Ca/HCO_3 type groundwaters (Seneca Army Depot Activity and Dover AFB) and the high salinity Dugway groundwaters (see Appendix B). However, the value of the pH_{zpc} is unknown and would have to be researched.

When developing mulch formulations, an iron mineral with a low pH_{zpc} should be selected for an iron source, due to the lower likelihood that iron sulfide coatings will form. Should additional iron sulfide nucleation sites be required, then an iron mineral with a high pH_{zpc} (which would form iron sulfide coatings) should be selected.

4.4 Analytical Techniques for Biowall Design and Evaluating System Performance

There is currently limited guidance for predicting the effectiveness of biogeochemical transformation of chlorinated solvents in groundwater. Therefore, evaluating the occurrence and significance of biogeochemical transformation may require an extensive list of environmental analyses, as well analyses not traditionally used in environmental remediation (e.g., electron microprobe). This data is likely to be necessary for the design of engineered systems that attempt to stimulate the formation of reactive iron sulfides *in situ*.

The analyses for evaluating systems for *in situ* biogeochemical transformation can be categorized as pre-design and operational as described below.

4.4.1 Pre-Design Testing

The pre-design analyses would include the following:

- Total organic carbon, and fractions of lignin, cellulose and hemicellulose in materials that might be used as mulch in the biowalls.
- Bench-scale testing of different substrate mixtures using site groundwater and the best mulch mix candidates based on the carbon analyses. The testing would consist of jar tests containing the substrate and site groundwater. The water would be analyzed for chlorinated ethenes, pH, Eh, dissolved oxygen, sulfide, sulfate and methane over time.
- Pilot-scale testing (to confirm bench-scale results)

4.4.1.1 Total Organic Carbon, Lignin, Cellulose, and Hemicellulose

The analyses of the total organic carbon and fractions of lignin, cellulose, and hemicellulose would provide information not only on how much organic carbon is provided by the substrate, but what fraction of the total organic carbon could be more easily converted to forms that could be utilized by sulfate-reducing bacteria. Such testing should be one of the first steps in selecting mulch for a biowall application.

4.4.1.2 Bench-Scale Testing

Bench-scale testing would involve testing the materials with lower lignin content in a series of microcosm tests. A specified mass of each of the proposed substrates would be placed in serum bottles with a given volume of site groundwater. After measuring initial chlorinated ethenes, temperature, E_h , pH, methane, and sulfate, of the groundwater, the bottles would then be sealed to maintain anaerobic conditions. Field parameters (temperature, E_h , pH, and sulfide), would then be measured periodically. Observations such as the presence or absence of hydrogen sulfide are also noted. At the end of the test the solutions would be analyzed for chlorinated ethene, methane, and sulfate concentrations for comparison to the original groundwater. Using the sulfate mass balance, and the duration of the test, a sulfide production rate for each proposed substrate would then be determined. In addition, a chlorinated ethene degradation rate constant would be calculated. Other information, such as a decrease in pH over the course of the test would be an indication that fermentation is taking place. Analyses could also be performed for the concentrations of useable forms of organic carbon, such as organic acids and alcohols. In this way, the systems could be fairly well understood under static conditions and the substrates which do the best job of promoting sulfate reduction could be selected for further testing.

Additional information could then be determined using a column test similar to the testing performed by Shen and Wilson (2007). The column tests provide information on reaction rates under flowing conditions, which is a more realistic than the microcosm test. Favorable column testing using a given substrate would then allow the pilot- or barrel-scale system to be designed. The optimum residence time would be known, so that wall thickness could be determined for a given groundwater velocity. The physical properties, such as the porosity and permeability of the substrate, should also be measured during the column test so that accurate residence times could be determined. Often, a conservative chemical such as bromide is added to columns to allow residence times to be determined. Although column tests provide more information than jar tests, they tend to be more labor intensive and expensive than jar tests.

4.4.1.3 Pilot-Scale Testing

Two to three of the best performing substrates from the jar and/or column testing should then be tested at the pilot- or barrel-scale. A barrel study consists of a series of barrels which have been plumbed with an influent fitting near the bottom and an effluent fitting near the top of the barrel. The barrel is then filled with the substrate to be tested. Barrel-scale tests are operated at the site and are operated under field conditions, such as temperature. Barrel tests are also significantly cheaper than pilot systems as no excavation is involved and the materials can be purchased inexpensively from the nearest hardware store.

Should the barrel-scale tests prove to be successful, then the more expensive field system (pilot or full-scale) can be installed.

4.4.2 Operational Testing

In order to evaluate system performance, many of the tests performed for this investigation are recommended, including:

- General Parameters (E_h , pH, dissolved oxygen, sulfide)

- Anions/Cations (and associated modeling)
- VOCs
- Ethanol and acetate
- Methane, ethene, ethane, and acetylene
- AVS/CrRS
- Electron microprobe (on samples where AVS+CrRS > 200 mg-S/kg)

4.4.2.1 General Parameters

The general parameters consisted of pH, oxidation-reduction potential, dissolved oxygen, specific conductance, temperature, ferrous iron, manganese, sulfide, alkalinity, total dissolved solids, and total organic carbon (preferably dissolved organic carbon). The field parameters (especially sulfide, E_h -sulfate/sulfide and pH) are an important first set of criteria for determining if conditions are favorable for the production of iron sulfides. However, these parameters can all be optimal and the system may still not meet expectations (i.e., Dugway Proving Ground and Seneca Army Depot Activity). Therefore, additional parameters need to be measured and evaluated.

4.4.2.2 Anions/Cations

The sulfate analysis is probably the most important parameter of the anion/cation analyses. The volumetric sulfate loading rate is an important factor in determining whether sufficient electron acceptors will be provided to the sulfate-reducing bacteria. In order to determine if gypsum and iron sulfides are at saturation, geochemical modeling such as PHREEQC is very useful. One can also determine if siderite is at saturation and if the addition of this mineral would increase the ferrous iron concentrations enough to precipitate iron sulfides. The other anions and cations (as well as the general parameters) are required for geochemical modeling.

4.4.2.3 VOCs

Concentrations of VOC, up gradient, down gradient and within the reaction zone are critical for determining plume trends, overall degradation rates, and biotic versus abiotic degradation using total moles of VOCs.

4.4.2.4 Methane, Ethene, Ethane, and Acetylene

Methane, ethene, and ethane are useful as “footprint” compounds to identify the type of transformation (abiotic vs. biotic and methanogenic versus sulfidogenic activity). However, in the environment of a biowall where fermenters are a necessary component for the systems to work, acetylene does not survive for long and could probably be removed from the analyte list after a few initial results confirm that it is not present above the detection limit.

4.4.2.5 AVS/CrRS

AVS/CrRS analysis is a practical tool to assess the concentrations of two “pools” of reactive iron sulfides. These concentrations can be used to calculate ranges of potential *in situ* contaminant transformation rates when used in combination with reliable rate constants from the literature. The analyses can also be used to select samples for more intensive analysis such as electron microprobe described below. Because the practical “detection limit” for finding iron sulfide

grains is about 200 mg/kg (AVS + CrRS) for a typical electron microprobe scan, only samples above this threshold should be selected for analysis.

4.4.2.6 Electron Microprobe

One of the most useful results of the electron microprobe analyses was the ability to determine the grain sizes and morphology of the iron sulfide (granular versus framboidal), which appears to be one of the most critical factors influencing the abiotic rate constant. The main limitations of the electron microprobe technique was the heterogeneity of the samples, which made it difficult to find phases that the AVS/CrRS indicated should be present and the difficulty in distinguishing the iron sulfide stoichiometries which are close to each other. Greigite, with 43 percent sulfur is very close to iron disulfide with 46.6 percent sulfur. On relatively large grains ($>2\ \mu\text{m}$), where the $1\text{-}2\ \mu\text{m}$ electron beam can be focused completely on the grain, distinguishing a 3.6 percent difference in sulfur content is possible, but for a $1\ \mu\text{m}$ grain the analysis tend to be diluted by the epoxy grain mount. Nevertheless, electron microprobe analysis can be a relatively inexpensive means to identify median grain sizes, mineral compositions, and morphologies.

4.4.3 Additional Parameters

Other parameters which were not evaluated, but may prove to be very useful include the following:

- X-ray diffraction, following grinding and magnetic or gravity separation.
- Polymerase chain reaction testing to obtain the fractions of and types of bacteria (sulfate-reducing bacteria, methanogens, fermenters, respiratory dechlorinators, etc.). A methodology is provided by Pruden et al. (2007).

4.4.3.1 X-Ray Diffraction

X-Ray diffraction may be able to fill the data gap left by the electron microprobe and AVS/CrRS analyses, namely the identification of the phases based on the crystal structure. However, due to the fairly low content of iron sulfides in some of the samples, concentration using magnetic or gravity methods may be required, which would mean the sample would have to be dried and ground, which would expose the iron sulfides to the atmosphere where oxidation could occur. Oxidation concerns were the main reason that this method was not selected for this investigation. However, assuming that at least a core of the original mineral would remain, it should be possible to obtain x-ray diffraction lines and identify the mineral present.

4.4.3.2 PCR

Polymerase chain reaction is a method that has recently been adapted to quantifying dechlorinating bacteria such as *Dehalococcoides* (USEPA, 2006; Lu et al., 2006a; Lu et al., 2006b) sulfate-reducing bacteria, methanogens, and fermenters, as well as other important bacteria such as *Thiobacillus denitrificans* within sulfate-reducing passive treatment systems (Pruden, 2007). Specific genes common to each type of bacteria are targeted and analyzed using PCR and other methodologies. The presence, concentrations, and activity of dechlorinating bacteria can be used to establish the relative contribution of purely biological contaminant degradation compared to biogeochemical transformation. The types and concentrations of sulfate-reducing bacteria can be used to determine the potential for sulfide generation which is required for biogeochemical iron sulfide production. Polymerase chain reaction holds the

promise of allowing complicated systems to be understood to a degree that has never been possible in the past.

4.5 Conclusions

The primary conclusions from this evaluation are as follows:

- The iron phases that were detected using the electron microprobe included iron minerals such as magnetite and hematite and various iron sulfides. The data also indicated that several iron sulfides were partially oxidized. The relative concentrations of total iron sulfides estimated by chemical extraction were generally consistent with the electron microprobe analysis results based on an estimated electron microprobe detection limit of about 200 mg/kg. These data indicate that the electron microprobe was a useful tool for identifying specific iron oxides and iron sulfides.
- The specific reactivity of framboidal pyrite may in fact have similar reactivity than iron monosulfide for a constant surface area. Thus the universe of iron sulfides responsible for in situ biogeochemical transformation of chlorinated ethenes appears to be broader than iron monosulfide.
- Geochemical modeling indicated that in general, iron oxides (e.g., magnetite and hematite) were undersaturated and thus could be expected to dissolve, and that iron sulfides (e.g., mackinawite, marcasite, troilite, greigite, and pyrite) were generally saturated or supersaturated and thus could be anticipated to form solid precipitates. Geochemical modeling provided an increased understanding of the potential to form specific reactive minerals and how these minerals would form at a given site. This understanding is important with respect to being able to design in situ biogeochemical transformation treatment systems because the specific mineral type and form directly control the rate of contaminant destruction. These data indicate that the presence of iron sulfides alone is insufficient to promote biogeochemical transformation.
- pH is very important with respect to controlling surface sites for the formation of iron sulfides and with respect to iron sulfide reactivity. Iron oxide minerals such as magnetite (at pH < 8.5) and hematite (at pH < 6.7) can provide surface sites for the formation of iron sulfides. Also, an increase in the pH from 6 to 8 can increase the rate constant by a factor of 5. The addition of specific iron oxides to the mulch can have a beneficial effect on biogeochemical transformation but must take aquifer pH into consideration.
- High chlorinated ethene biogeochemical transformation rate is dependent on both the presence of iron sulfides and a high volumetric sulfate loading rate to the biowall. A low volumetric sulfate loading rate leads to low sulfide production rates and can result in the rate of active iron sulfide formation being outweighed by the rate of active iron sulfide aging to less reactive forms such as greigite. Sufficient organic carbon in combination with a high volumetric sulfate loading rate and a source of biologically or chemically reducible ferric iron appear to be critical factors that promote the ongoing production of high surface area iron sulfide minerals that drive in situ biogeochemical transformation processes. The presence of iron sulfides alone is insufficient to promote biogeochemical transformation.

- Another important factor in maximizing the rate of reaction between chlorinated ethenes and iron sulfides is the surface area of the iron sulfides. A decrease in the median grain size of the iron sulfide particles from 1 μm to 10 nm can increase the rate constant by 100 times. Although nanoparticles were not likely present in any of the field systems investigated in this study, several investigators have reported the production of nanoparticulate iron monosulfides by sulfate-reducing bacteria (Ohfuji and Rickard, 2006). Ostwald ripening can result in the loss of mineral surface area and reactivity and can be caused by infiltration of surface water into a biowall. Surface water infiltration can also lead to iron sulfide oxidation and loss of reactivity. Maintaining a dynamic system with a high volumetric sulfate flux is critical.
- The factors which were identified in this study as important for in situ biogeochemical transformation of chlorinated ethenes include reduced iron phase mineralogy, iron oxide mineralogy, volumetric sulfate loading rate and organic carbon content. These factors should be considered when designing *in situ* biogeochemical transformation systems for remediation of chlorinated ethenes.

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Appendix A
Soil Analysis Raw Data Reports

Acid-Volatile Sulfide and Chromium-Reducible Sulfide Data

Altus Sites OU-1 and SS-17

9/28/2007

H2O content in Altus freeze cores

	tube wt (g)	tube+wet sample(g)	tube+dry sample(g)	wet sample(g)	dry sample(g)	H2O%	Mean H2O%
EPA-C1a	21.443	29.516	27.1155	8.073	5.6725	29.73	28.64
EPA-C1b	21.551	31.73	28.9261	10.179	7.3751	27.55	
EPA-C3a	21.453	27.545	24.8841	6.092	3.4311	43.68	50.22
EPA-C3b	21.563	27.559	24.1556	5.996	2.5926	56.76	
EPA-C4a	21.583	26.8	24.7417	5.217	3.1587	39.45	37.98
EPA-C4b	21.664	30.589	27.331	8.925	5.667	36.50	
EPA-C5a	21.381	28.935	26.1279	7.554	4.7469	37.16	37.78
EPA-C5b	21.554	28.787	26.0096	7.233	4.4556	38.40	
EPA-C6a	21.584	30.958	27.6141	9.374	6.0301	35.67	39.07
EPA-C6b	21.771	30.009	26.5097	8.238	4.7387	42.48	
EPA-C7a	21.318	32.12	28.5181	10.802	7.2001	33.34	35.09
EPA-C7b	21.379	30.102	26.8892	8.723	5.5102	36.83	
EPA-C11a	21.646	29.942	27.1345	8.296	5.4885	33.84	33.83
EPA-C11b	21.41	30.492	27.42	9.082	6.01	33.83	
EPA-C13a	21.411	30.482	26.9881	9.071	5.5771	38.52	33.52
EPA-C13b	21.81	31.759	28.9206	9.949	7.1106	28.53	
EPA-C13aa	21.54	32.369	28.7575	10.829	7.2175	33.35	26.53
EPA-C13ab	21.642	34.559	32.0137	12.917	10.3717	19.71	
EPA-C15a	22.03	33.414	30.0309	11.384	8.0009	29.72	27.50
EPA-C15b	21.78	35.527	32.0521	13.747	10.2721	25.28	
EPA-C15aa	21.575	33.872	30.1028	12.297	8.5278	30.65	30.65
EPA-C15ab	21.785	31.601	27.1886	9.816	5.4036	44.95	*loss of sample

AVS measurement
9/27/2007

	wet sample(g)	Mean H2O%	dry sample (g)	ugS	AVS (mg/kg)	AVS mean (mg/kg)	stdev
EPA-C1a	3.822	28.64	2.7274	966.76	354.47	490.10	138.00
EPA-C1b	1.377	28.64	0.9826	619.39	630.34		
EPA-c1c	5.07	28.64	3.6179	1756.5	485.50		
EPA-C3a	2.342	50.22	1.1659	107.7	92.38	108.63	22.98
EPA-C3b	3.638	50.22	1.8110	226.15	124.88		
EPA-C4a	3.54	37.98	2.1955	287.36	130.88	163.54	46.18
EPA-C4b	4.79	37.98	2.9708	582.85	196.20		
EPA-C5a	2.203	37.78	1.3707	433.55	316.30	366.17	70.54
EPA-C5b	3.087	37.78	1.9207	799.12	416.05		
EPA-C6a	3.11	39.07	1.8948	502.02	264.95	232.53	45.84
EPA-C6b	2.319	39.07	1.4130	282.76	200.12		
EPA-C7a	3.271	35.09	2.1233	554.89	261.34	219.00	59.88
EPA-C7b	2.884	35.09	1.8720	330.7	176.66		
EPA-C11a	6.932	33.83	4.5867	1473.2	321.19	350.52	41.48
EPA-C11b	5.541	33.83	3.6665	1392.72	379.85		
EPA-C13a	5.902	33.52	3.9235	505.01	128.72	130.79	2.93
EPA-C13b	3.848	33.52	2.5582	339.87	132.86		
EPA-C13aa	9.105	26.53	6.6897	1296.24	193.77	192.16	2.27
EPA-C13ab	4.365	26.53	3.2070	611.12	190.56		
EPA-C15a	5.732	27.50	4.1558	543.33	130.74	155.95	35.65
EPA-C15b	4.324	27.50	3.1349	567.92	181.16		
EPA-C15aa	8.12	30.65	5.6311	1237.6	219.78	252.69	46.54
EPA-C15ab	4.613	30.65	3.1991	913.65	285.59		

Total Fe, S by digestion

Field Sample ID	Sulfur (S) mg/kg	S mean (mg/kg)
LKSD 1	13100	
LKSD 1	12900 (RPD=1.54)	
ES-SED 1	2440	
EPA-C1	463	476.33
EPA-C1B	435	
EPA-C1B	531	
EPA-C3	146	147.00
EPA-C3	148	
EPA-C4	274	393.00
EPA-C4B	512	
EPA-C5	441	506.00
EPA-C5B	571	
EPA-C6	526	498.50
EPA-C6B	471	
EPA-C7	696	698.33
EPA-C7B	696	
EPA-C7B	703	
EPA-C11	ND	39.90
EPA-C11B	39.9	
EPA-C13	42.0	42.00
EPA-C13A	ND	
EPA-C13A	ND	
EPA-C15	127	127.00
EPA-C15A	84.4	84.40

SO4 extraction
20ml 2.4mM NaHCO3, 2.6mM Na2CO3 extract 24h

	wet sample(g)	Mean H2O%	wet wt(g)	dry wt (g)	SO4 (mg/L)	SO4 (mg/kg)	SO4 mean (mg/kg)
EPA-C1a	4.045	28.64	1.505	1.0740	1.94	36.13	39.74
EPA-C1b	3.513	28.64	2.955	2.1087	4.57	43.34	
EPA-C3a	3.388	50.22	1.968	0.9797	6.17	125.96	103.98
EPA-C3b		50.22	1.323	0.6586	2.7	81.99	
EPA-C4a	5.089	37.98	2.219	1.3762	2.83	41.13	32.79
EPA-C4b		37.98	1.714	1.0630	1.3	24.46	
EPA-C5a	2.981	37.78	1.609	1.0011	2.83	56.54	48.73
EPA-C5b		37.78	1.634	1.0167	2.08	40.92	
EPA-C6a	2.33	39.07	1.399	0.8523	2.01	47.16	53.92
EPA-C6b		39.07	1.623	0.9889	3	60.67	
EPA-C7a	3.271	35.09	1.416	0.9192	4.01	87.25	92.03
EPA-C7b		35.09	1.149	0.7458	3.61	96.81	
EPA-C11a	3.062	33.83	1.408	0.9316	3.4	72.99	65.09
EPA-C11b		33.83	1.665	1.1017	3.15	57.18	
EPA-C13a	6.057	33.52	1.699	1.1294	2.74	48.52	32.49
EPA-C13b		33.52	3.307	2.1985	1.81	16.47	
EPA-C13aa	4.123	26.53	2.435	1.7891	2.9	32.42	35.63
EPA-C13ab		26.53	1.598	1.1741	2.28	38.84	
EPA-C15a	3.181	27.50	2.061	1.4943	2.63	35.20	34.87
EPA-C15b		27.50	1.765	1.2796	2.21	34.54	
EPA-C15aa	3.12	30.65	2.118	1.4688	6.5	88.51	85.40
EPA-C15ab		30.65	1.703	1.1810	4.86	82.30	
lksd1				0.2598	44.2	3402.62	
lksd2				0.1698	29.4	3462.90	

CRS measurement

			dry sample		CRS	CRS mean		TRS		
	wet sample(g)	Mean H2O%	(g)	ugS	(mg/kg)	(mg/kg)	stdev	mean	AVS mean	CRS
								(mg/kg)	(mg/kg)	(mg/kg)
EPA-C1a	4.045	28.64	2.8865	1985.99	688.03	617.44	99.82	617.44	490.10	127.34
EPA-C1b	3.513	28.64	2.5069	1370.89	546.86					
EPA-C3a	3.388	50.22	1.6866	722.05	428.12	428.12		428.12	108.63	319.49
EPA-C3b		50.22								
EPA-C4a	5.089	37.98	3.1563	1446.03	458.15	458.15		458.15	163.54	294.61
EPA-C4b		37.98								
EPA-C5a	2.981	37.78	1.8548	1345.01	725.16	725.16		725.16	366.17	358.98
EPA-C5b		37.78								
EPA-C6a	2.33	39.07	1.4196	699.04	508.64	508.64		508.64	232.53	276.11
EPA-C6b		39.07								
EPA-C7a	3.271	35.09	2.1233	865.27	407.52	407.52		407.52	219.00	188.52
EPA-C7b		35.09								
EPA-C11a	3.062	33.83	2.0260	754.11	372.21	372.21		372.21	350.52	21.69
EPA-C11b		33.83								
EPA-C13a	6.057	33.52	4.0265	541.61	134.51	134.51		134.51	130.79	3.72
EPA-C13b		33.52								
EPA-C13aa	4.123	26.53	3.0293	653.8	215.83	215.83		215.83	192.16	23.66
EPA-C13ab		26.53								
EPA-C15a	3.181	27.50	2.3063	464.05	201.21	201.21		201.21	155.95	45.26
EPA-C15b		27.50								
EPA-C15aa	3.12	30.65	2.1637	432.64	199.96	199.96		199.96	252.69	-52.73
EPA-C15ab		30.65								

TABLE 6
SUMMARY OF SOIL/MULCH ANALYTICAL RESULTS
OU-1 BIOWALL DEMONSTRATION
ALTUS AFB, OKLAHOMA

Sample Location	Sample Date	Sample ID	Sample Depth (feet bgs) ^{a/}	Percent Solids	(mg/kg)	(mg/kg)	(mg/kg)	WAE Fe ²⁺ ^{c/} (mg/kg)	SAE Fe ²⁺ ^{c/} (mg/kg)	AVS ^{c/} (mg/kg)	CES ^{b/} (mg/kg)
BB04W		bbo4w-a								410	1,109
		bbo4w-b								ND	110
BB05W		bbo5w-a								295	520
		bbo5w-b								61	218
BB07W		bb07w-a								165	357
		bbo7w-b								301	353
BF12W		bf12w-a								ND	49
		bf12w-b								ND	46

^{a/} feet bgs = feet below ground surface.

^{b/} mg/kg = micrograms per kilogram dry weight.

^{c/} Bio Fe³⁺ = bioavailable ferric iron; Bio Mn = bioavailable manganese; WAE Fe²⁺ = weak acid extractable ferrous iron;

SAE Fe²⁺ = strong acid extractable ferrous iron; SAE Mn = strong acid extractable divalent manganese;

AVS = acid volatile sulfide; CES = chromium extractable sulfide.

EPA Column Study (Altus Site SS-17)

freeze dry wt

**B3 slice X
sect 1C**

	tube wt (g)	tube+wet wt	tube +dry wt	H2O content(g)	solid wt	H2O %
1	10.337	64.96	42.368	22.592	32.031	41.36
2	10.287	71.91	47.185	24.725	36.898	40.12
3	10.368	76.77	56.431	20.339	46.063	30.63
4	10.384	77.64	53.162	24.478	42.778	36.40
5	10.327	78.54	56.405	22.135	46.078	32.45
6	10.283	82.04	58.18	23.860	47.897	33.25
7	10.345	77.14	56.571	20.569	46.226	30.79
8	10.324	79.26	57.511	21.749	47.187	31.55
9	10.353	77.13	54.528	22.602	44.175	33.85

AVS measurement

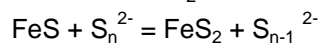
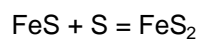
AVS using freeze dry samples

B3 slice X sect 1	sample wt(g)	AVS (ppm)		Mean	stdev
1	0.537	793.18		793.18	#DIV/0!
2	0.753	1872	0.1872 %	1872.00	#DIV/0!
3	0.691	1604	0.1604 %	1364.26	339.05
4	0.678	1124.51			
	0.535	1321.8		1321.80	#DIV/0!
5	0.815	1501.19		1501.19	#DIV/0!
6	0.644	798.1		798.10	#DIV/0!
7	0.517	1041.16		914.99	178.44
	0.951	788.81			
8	0.771	853.6		847.57	8.53
	1.223	841.54			
9	0.693	508.83		468.49	57.06
	0.696	428.14			

AVS using wet samples

B3 slice X sect 1	wet sample wt(g)	H2O %	sample wt (g)	S (ugs)	AVS (ppm)		Mean	stdev
1	2.343	0.35	1.5230	1446.44	949.761975		1020.54	100.09
	2.372	0.35	1.5418	1682.58	1091.30886			
2	3.312	0.35	2.1528	6255.54	2905.76923	0.2905 %	2642.84	371.83
	2.413	0.35	1.5685	3732.78	2379.91648			
3	2.456	0.35	1.5964	3218.34	2015.9985	0.2015 %	2087.98	101.80
	4.132	0.35	2.6858	5801.23	2159.96351			
4	2.639	0.35	1.7154	3475.38	2026.04716		2158.40	187.17
	2.795	0.35	1.8168	4161.72	2290.74997			
5	3.456	0.35	2.2464	3543.31	1577.32817		1630.14	74.68
	2.94	0.35	1.9110	3216.11	1682.9461			
6	3.682	0.35	2.3933	3728.36	1557.83228		1449.56	153.12
	3.835	0.35	2.4928	3343.51	1341.29375			
7	3.032	0.35	1.9708	2873.43	1458.00183		1295.54	229.76
	3.961	0.35	2.5747	2917.26	1133.07051			
8	2.161	0.35	1.4047	1441.44	1026.19158		1190.06	231.74
	3.256	0.35	2.1164	2865.44	1353.92175			
9	2.158	0.35	1.4027	734	523.276538		577.45	76.61
	3.448	0.35	2.2412	1415.58	631.616991			

B3 slice X sect 1	measured CRS			AVS-CRS	time	AVS to CRS
	AVS	AVS+CRS	CRS	%converted	t(day)	k(mol kg ⁻¹) (d ⁻¹)
1	1020.54	3795.53	2774.99	73.11	793.00	0.00166
2	2642.84	2747.71	104.87	3.82	793.00	0.00005
3	2087.98	2618.25	530.27	20.25	793.00	0.00029
4	2158.40	4278.84	2120.44	49.56	793.00	0.00086
5	1630.14	2617.22	987.08	37.71	793.00	0.00060
6	1449.56	2967.37	1517.81	51.15	793.00	0.00090
7	1295.54	3088.81	1793.27	58.06	793.00	0.00110
8	1190.06	2145.21	955.15	44.52	793.00	0.00074
9	577.45	2160.63	1583.18	73.27	793.00	0.00166



C is AVS concentration

$-dC/dt = kSC$ Assume S constant

Integrate

$$\ln C_0 - \ln C = kSt$$

$$k = (\ln C_0 - \ln C)/t$$

C₀=initial conc. AVS

C=final conc. AVS

6/25/2007

CRS using wet samples

B3 slice X		sample		sample		CRS	CRS Mean	
sect 1		wt(g)	H2O %	wt (g)	measured S (ugs)	(ppm)	(ppm)	stdev
1		3.551	0.35	2.3082	5760.40	2495.68	3795.53	1251.77
		2.297	0.35	1.4931	4566.48	3058.49		
		1.614	0.35	1.0491	4584.99	4370.40		
		2.122	0.35	1.3793	7251.73	5257.54		
2		2.968	0.35	1.9292	6120.24	3172.42	2747.71	439.36
		3.91	0.35	2.5415	5832.75	2295.00		
		3.674	0.35	2.3881	7337.85	3072.67		
		3.468	0.35	2.2542	5524.46	2450.74		
3		3.869	0.35	2.5149	5882.86	2339.25	2618.25	508.80
		4.012	0.35	2.6078	8359.33	3205.51		
		3.95	0.35	2.5675	5930.88	2309.98		
4		3.611	0.35	2.3472	9116.80	3884.20	4278.84	740.39
		2.999	0.35	1.9494	10005.91	5132.95		
		1.928	0.35	1.2532	4786.45	3819.38		
5		4.124	0.35	2.6806	6158.14	2297.30	2617.22	550.07
		2.784	0.35	1.8096	5885.51	3252.38		
		2.934	0.35	1.9071	4390.08	2301.97		
6		3.891	0.35	2.5292	7736.98	3059.12	2967.37	129.75
		2.962	0.35	1.9253	5536.44	2875.62		
7		4.682	0.35	3.0433	6677.19	2194.06	3088.81	926.66
		3.222	0.35	2.0943	8470.16	4044.39		
		2.776	0.35	1.8044	5463.68	3027.98		
8		4.044	0.35	2.6286	4814.79	1831.69	2145.21	673.30
		3.341	0.35	2.1717	6337.07	2918.09		
		4.319	0.35	2.8074	4732.72	1685.83		
9		2.982	0.35	1.9383	3102.57	1600.67	2160.63	791.90
		3.039	0.35	1.9754	5374.11	2720.59		
reference material								
lake sediment 1				0.5226	4979.51	0.9528 %		
lake sediment 2				0.454	4215.90	0.9286 %		
esturine sediment				0.4295	1085.34	0.2527 %		

Dover AFB

H2O content determination in Dover sediments

Sample	location	bottle wt(g)	bottle+wet wt(g)	bottle+dry wt(g)	H2O %	Mean H2O %	stdev
TSB1-10a		21.239	24.184	23.448	24.99	27.54	3.61
TSB1-10b		21.585	24.343	23.513	30.09		
TSB1-17a		21.389	25.072	24.184	24.11	24.54	0.61
TSB1-17b		21.627	24.042	23.439	24.97		
TSB3-10a		21.472	24.9	23.883	29.67	29.04	0.89
TSB3-10b		21.338	25.837	24.559	28.41		
TSB3-16a		21.435	24.751	23.794	28.86	29.02	0.23
TSB3-16b		21.39	24.806	23.809	29.19		
TSB6-10a		21.549	24.886	23.731	34.61	28.12	9.18
TSB6-10b		21.612	25.685	24.804	21.63		
TSB6-17a		21.701	26.418	25.058	28.83	28.99	0.22
TSB6-17b		21.365	24.927	23.889	29.14		
TSB8-10a		21.751	25.89	25.019	21.04	24.77	5.27
TSB8-10b		21.671	26.363	25.026	28.50		
TSB8-17a		21.449	26.069	24.965	23.90	24.82	1.30
TSB8-17b		21.585	25.579	24.551	25.74		

AVS and CRS determination in Dover sediments

Sample	location	wet wt(g)	H2O %	dry wt	AVS-S (ugS)	AVS (mg/kg)	AVS-mean (mg/kg)	AVS stdev	CRS-S (ugS)	CRS (mg/kg)	CRS-mean (mg/kg)	CRS stdev
TSB1-10a		3.618	27.54	2.621498	411.25	156.88	301.57	204.63	394.36	150.43	176.08	36.27
TSB1-10b		3.81	27.54	2.760616	1231.96	446.26			556.9	201.73		
TSB1-17a		2.189	24.54	1.651822	1104.4	668.59	580.65	124.37	437.56	264.90	259.95	6.99
TSB1-17b		2.659	24.54	2.006485	988.61	492.71			511.66	255.00		
TSB3-10a		3.175	29.04	2.253079	1937.13	859.77	821.22	54.52	654.52	290.50	285.57	6.98
TSB3-10b		4.039	29.04	2.8662	2243.28	782.67			804.35	280.63		
TSB3-16a		5.81	29.02	4.123756	799.66	193.92	169.02	35.21	373.08	90.47	113.95	33.21
TSB3-16b		3.044	29.02	2.160536	311.37	144.12			296.94	137.44		
TSB6-10a		2.664	28.12	1.914854	3174.37	1657.76	1419.94	336.33	2766.11	1444.55	1591.55	207.88
TSB6-10b		2.479	28.12	1.781878	2106.38	1182.11			3097.87	1738.54		
TSB6-17a		2.598	28.99	1.844933	2723.45	1476.18	1538.56	88.22	2272.28	1231.63	1315.34	118.37
TSB6-17b		2.592	28.99	1.840672	2946.81	1600.94			2575.17	1399.04		
TSB8-10a		2.199	24.77	1.654318	1706.82	1031.74	1104.75	103.25	2339.02	1413.89	2113.84	989.89
TSB8-10b		1.421	24.77	1.069025	1259.05	1177.76			3008.02	2813.80		
TSB8-17a		2.389	24.82	1.796113	2460.75	1370.04	1408.05	53.75	1820.39	1013.52	1049.74	51.23
TSB8-17b		2.349	24.82	1.76604	2553.79	1446.05			1917.86	1085.97		

Seneca Depot

H2O content determination in Seneca sediments

Sample	location	bottle wt(g)	bottle+wet wt(g)	bottle+dry wt(g)	H2O %	Mean H2O %	stdev
Seneca A1a	6.0-8.0	21.665	29.17	27.194	26.33	28.67	3.31
Seneca A1b		21.469	25.767	24.434	31.01		
Seneca A1	9.0-11.0	21.314	27.922	26.21	25.91	26.12	0.30
Seneca A2		21.816	25.28	24.368	26.33		
Seneca B1a	7.0-9.0	21.632	26.984	25.636	25.19	24.39	1.12
Seneca B1b		21.722	27.891	26.435	23.60		
Seneca B1a	9.5-7.5	21.672	25.93	24.71	28.65	29.78	1.59
Seneca B1b		21.879	27.944	26.07	30.90		

AVS and CRS determination in Dover sediments

Sample	location	wet wt(g)	H2O %	dry wt	AVS-S (ugS)	AVS (mg/kg)	AVS-mean (mg/kg)	AVS stdev	CRS-S (ugS)	CRS (mg/kg)	CRS-mean (mg/kg)	CRS stdev
Seneca A1a	6.0-8.0	2.72	28.67	1.940128	168.02	86.60	62.72	33.77	375.79	193.69	205.22	16.30
Seneca A1b		4.33	28.67	3.088512	119.96	38.84			669.43	216.75		
Seneca A1	9.0-11.0	4.148	26.12	3.064627	142.72	46.57	64.83	25.83	484.48	158.09	156.99	1.55
Seneca A2		3.899	26.12	2.88066	239.37	83.10			449.08	155.89		
Seneca B1a	7.0-9.0	3.404	24.39	2.573616	70.84	27.53	18.14	13.28	566.05	219.94	197.45	31.81
Seneca B1b		3.868	24.39	2.924426	25.59	8.75			511.65	174.96		
Seneca B1a	9.5-7.5	2.86	29.78	2.008427	52.14	25.96	23.15	3.97	351.79	175.16	175.16	#DIV/0!
Seneca B1b		2.96	29.78	2.078652	42.29	20.34						

Dugway PG

H2O content determination in Dugway sediments

Sample	location	bottle wt(g)	bottle+wet wt(g)	bottle+dry wt(g)	H2O %	Mean H2O %	stdev
FD90a		22.174	24.74	24.309	16.80	16.79	0.01
FD90b		22.154	24.663	24.242	16.78		
SO86a		21.576	25.213	24.702	14.05	14.08	0.05
SO86b		21.914	25.449	24.95	14.12		
SO87a		21.505	25.218	24.663	14.95	14.70	0.35
SO87b		21.327	23.804	23.446	14.45		
SO88a		21.716	26.221	25.523	15.49	15.49	0.00
SO88b		21.716	26.221	25.523	15.49		
SO89a		21.542	25.208	24.589	16.88	17.10	0.30
SO89b		21.697	25.544	24.878	17.31		
SO90a		21.392	25.348	24.644	17.80	18.42	0.88
SO90b		21.962	25.108	24.509	19.04		
SO91a		21.52	24.989	24.543	12.86	12.89	0.05
SO91b		21.339	24.179	23.812	12.92		

AVS and CRS determination in Dugway sediments

Sample	location	wet wt(g)	H2O %	dry wt	AVS-S (ugS)	AVS (mg/kg)	AVS-mean (mg/kg)	AVS stdev	CRS-S (ugS)	CRS (mg/kg)	CRS-mean (mg/kg)	CRS stdev
FD90a		5.009	16.79	4.168085	459.61	110.27	112.46	3.10	159.51	38.27	43.29	7.11
FD90b		3.442	16.79	2.864154	328.38	114.65			138.39	48.32		
SO86a		2.76	14.08	2.371309	7.67	3.23	3.23		0.5	0.21	0.21	
SO87a		4.16	14.70	3.548471	69.09	19.47	19.47		242.3	68.28	68.28	
SO88a		2.798	15.49	2.364481	429.16	181.50	181.50		264.59	111.90	111.90	
SO89a		2.817	17.10	2.335334	216.92	92.89	92.89		1.6	0.69	0.69	
SO90a		5.359	18.42	4.371985	351.82	80.47	80.47		123.76	28.31	28.31	
SO91a		2.056	12.89	1.790989	55.41	30.94	30.94		720.78	402.45	402.45	

Iron Extraction Data

Altus Sites OU-1 and SS-17

9/28/2007

H2O content in Altus freeze cores

	tube wt (g)	tube+wet sample(g)	tube+dry sample(g)	wet sample(g)	dry sample(g)	H2O%	Mean H2O%
EPA-C1a	21.443	29.516	27.1155	8.073	5.6725	29.73	28.64
EPA-C1b	21.551	31.73	28.9261	10.179	7.3751	27.55	
EPA-C3a	21.453	27.545	24.8841	6.092	3.4311	43.68	50.22
EPA-C3b	21.563	27.559	24.1556	5.996	2.5926	56.76	
EPA-C4a	21.583	26.8	24.7417	5.217	3.1587	39.45	37.98
EPA-C4b	21.664	30.589	27.331	8.925	5.667	36.50	
EPA-C5a	21.381	28.935	26.1279	7.554	4.7469	37.16	37.78
EPA-C5b	21.554	28.787	26.0096	7.233	4.4556	38.40	
EPA-C6a	21.584	30.958	27.6141	9.374	6.0301	35.67	39.07
EPA-C6b	21.771	30.009	26.5097	8.238	4.7387	42.48	
EPA-C7a	21.318	32.12	28.5181	10.802	7.2001	33.34	35.09
EPA-C7b	21.379	30.102	26.8892	8.723	5.5102	36.83	
EPA-C11a	21.646	29.942	27.1345	8.296	5.4885	33.84	33.83
EPA-C11b	21.41	30.492	27.42	9.082	6.01	33.83	
EPA-C13a	21.411	30.482	26.9881	9.071	5.5771	38.52	33.52
EPA-C13b	21.81	31.759	28.9206	9.949	7.1106	28.53	
EPA-C13aa	21.54	32.369	28.7575	10.829	7.2175	33.35	26.53
EPA-C13ab	21.642	34.559	32.0137	12.917	10.3717	19.71	
EPA-C15a	22.03	33.414	30.0309	11.384	8.0009	29.72	27.50
EPA-C15b	21.78	35.527	32.0521	13.747	10.2721	25.28	
EPA-C15aa	21.575	33.872	30.1028	12.297	8.5278	30.65	30.65
EPA-C15ab	21.785	31.601	27.1886	9.816	5.4036	44.95	*loss of sample

10/15/2007

10ml ascorbate extract for 24h.

H2O content in Altus freeze cores

	H2O%	Mean H2O%	wet sample (g)	dry wt(g)	ICP tot Fe (mg/L)	tot Fe (mg/kg)	mean Fe (mg/kg)
EPA-C1a	29.73	28.64	1.941	1.3851	7.89	56.96	59.54
EPA-C1b	27.55	28.64	1.55	1.1061	6.87	62.11	
EPA-C3a	43.68	50.22	1.245	0.6198	3.41	55.02	60.40
EPA-C3b	56.76	50.22	1.298	0.6461	4.25	65.77	
EPA-C4a	39.45	37.98	1.914	1.1871	5.14	43.30	40.72
EPA-C4b	36.50	37.98	1.708	1.0593	4.04	38.14	
EPA-C5a	37.16	37.78	1.619	1.0073	3.28	32.56	43.03
EPA-C5b	38.40	37.78	1.511	0.9401	5.03	53.50	
EPA-C6a	35.67	39.07	1.476	0.8993	9.52	105.87	99.34
EPA-C6b	42.48	39.07	1.252	0.7628	7.08	92.81	
EPA-C7a	33.34	35.09	1.506	0.9776	7.70	78.77	69.49
EPA-C7b	36.83	35.09	1.65	1.0710	6.45	60.22	
EPA-C11a	33.84	33.83	2.261	1.4960	23.9	159.76	162.86
EPA-C11b	33.83	33.83	2.058	1.3618	22.6	165.96	
EPA-C13a	38.52	33.52	1.207	0.8024	21.0	261.72	273.30
EPA-C13b	28.53	33.52	1.621	1.0776	30.7	284.88	
EPA-C13aa	33.35	26.53	2.034	1.4944	29.7	198.74	210.86
EPA-C13ab	19.71	26.53	2.057	1.5113	33.7	222.99	
EPA-C15a	29.72	27.50	2.015	1.4609	41.6	284.75	260.80
EPA-C15b	25.28	27.50	1.619	1.1738	27.8	236.84	
EPA-C15aa	30.65	30.65	1.631	1.1311	16.6	146.76	152.42
EPA-C15ab	44.95	30.65	1.87	1.2968	20.5	158.08	
LKSD1				0.3015	74.6	2474.30	
LKSD2				0.2777	69.1	2488.30	

10/15/2007

10ml dithionite extract for 4h at 60C

H2O content in Altus freeze cores

	H2O%	Mean H2O%	wet sample (g)	dry wt(g)	ICP tot Fe (mg/L)	tot Fe (mg/kg)	mean Fe (mg/kg)
EPA-C1a	29.73	28.64	1.73	1.2345	79.6	644.78	654.88
EPA-C1b	27.55	28.64	1.924	1.3730	91.3	664.98	
EPA-C3a	43.68	50.22	1.195	0.5949	48.3	811.94	701.17
EPA-C3b	56.76	50.22	1.919	0.9553	56.4	590.40	
EPA-C4a	39.45	37.98	1.627	1.0091	45.9	454.87	411.91
EPA-C4b	36.50	37.98	1.582	0.9812	36.2	368.95	
EPA-C5a	37.16	37.78	1.286	0.8002	59.3	741.11	783.90
EPA-C5b	38.40	37.78	1.357	0.8443	69.8	826.70	
EPA-C6a	35.67	39.07	1.562	0.9517	70.8	743.97	689.84
EPA-C6b	42.48	39.07	1.58	0.9627	61.2	635.72	
EPA-C7a	33.34	35.09	1.389	0.9016	60.0	665.46	712.55
EPA-C7b	36.83	35.09	1.229	0.7977	60.6	759.64	
EPA-C11a	33.84	33.83	1.582	1.0468	553	5282.99	6138.31
EPA-C11b	33.83	33.83	1.625	1.0753	752	6993.64	
EPA-C13a	38.52	33.52	1.627	1.0816	448	4142.11	3916.95
EPA-C13b	28.53	33.52	1.532	1.0185	376	3691.80	
EPA-C13aa	33.35	26.53	1.27	0.9331	558	5980.07	5625.52
EPA-C13ab	19.71	26.53	1.601	1.1763	620	5270.97	
EPA-C15a	29.72	27.50	2.007	1.4551	646	4439.50	4137.37
EPA-C15b	25.28	27.50	2.201	1.5957	612	3835.25	
EPA-C15aa	30.65	30.65	1.344	0.9320	521	5589.86	5167.63
EPA-C15ab	44.95	30.65	1.258	0.8724	414	4745.40	
LKSD1				0.1898	48.6	2560.59	
LKSD2				0.2949	83.5	2831.47	

Total Fe, S by digestion

Field Sample ID	Iron (Fe)	Mean Fe(mg/kg)
	mg/kg	
LKSD 1	20100	00 (RPD=1.00)
LKSD 1	00 (RPD=1.00)	
ES-SED 1	16400	2505
EPA-C1	2240	
EPA-C1B	2390	1270
EPA-C1B	2620	
EPA-C3	1270	1790
EPA-C3	1270	
EPA-C4	1560	2110
EPA-C4B	2020	
EPA-C5	1990	2775
EPA-C5B	2230	
EPA-C6	2690	2700
EPA-C6B	2860	
EPA-C7	2610	10755
EPA-C7B	2790	
EPA-C7B	2790	6070
EPA-C11	9210	
EPA-C11B	12300	11050
EPA-C13	6070	
EPA-C13A	11300	8260.0
EPA-C13A	10800	
EPA-C15	8260	8870
EPA-C15A	8870	

10/16/2007

10ml 0.5M HCl extract for 1h.

H2O content in Altus freeze cores

	H2O%	Mean H2O%	wet sample (g)	dry wt(g)	Fe2+ (mg/L)	dilution	Fe2+ (mg/L)	ICP tot Fe (mg/L)	Fe2+ (mg/kg)	tot Fe (mg/kg)	mean Fe (mg/kg)
EPA-C1a	29.73	28.64	2.285	1.6306	0.81	250	202.5	165	1241.90	1011.92	990.81
EPA-C1b	27.55	28.64	2.081	1.4850	0.68	250	170	144	1144.78	969.70	
EPA-C3a	43.68	50.22	1.551	0.7721	0.18	250	45	38.7	582.83	501.24	512.64
EPA-C3b	56.76	50.22	1.334	0.6641	0.15	250	37.5	34.8	564.70	524.04	
EPA-C4a	39.45	37.98	1.646	1.0209	0.21	250	52.5	46.0	514.27	450.60	476.79
EPA-C4b	36.50	37.98	1.808	1.1213	0.27	250	67.5	56.4	601.97	502.98	
EPA-C5a	37.16	37.78	1.132	0.7043	0.63	125	78.75	72.6	1118.08	1030.76	996.15
EPA-C5b	38.40	37.78	1.038	0.6458	0.56	125	70	62.1	1083.85	961.53	
EPA-C6a	35.67	39.07	1.283	0.7817	0.43	125	53.75	51.5	687.63	658.85	702.03
EPA-C6b	42.48	39.07	1.513	0.9219	0.59	125	73.75	68.7	800.00	745.22	
EPA-C7a	33.34	35.09	1.124	0.7296	0.41	125	51.25	46.0	702.43	630.47	697.88
EPA-C7b	36.83	35.09	1.23	0.7984	0.53	125	66.25	61.1	829.79	765.29	
EPA-C11a	33.84	33.83	2.031	1.3438	1.13	125	141.25	131	1051.09	974.82	1072.50
EPA-C11b	33.83	33.83	2.118	1.4015	1.43	125	178.75	164	1275.44	1170.19	
EPA-C13a	38.52	33.52	1.224	0.8137	0.54	125	67.5	64.1	829.57	787.78	1002.05
EPA-C13b	28.53	33.52	1.348	0.8962	0.94	125	117.5	109	1311.16	1216.31	
EPA-C13aa	33.35	26.53	1.832	1.3460	1.36	125	170	159	1262.99	1181.27	1189.33
EPA-C13ab	19.71	26.53	1.455	1.0690	1.07	125	133.75	128	1251.18	1197.39	
EPA-C15a	29.72	27.50	1.505	1.0912	0.9	125	112.5	101	1031.01	925.62	963.33
EPA-C15b	25.28	27.50	1.433	1.0389	0.92	125	115	104	1106.91	1001.03	
EPA-C15aa	30.65	30.65	2.173	1.5069	1.51	125	188.75	191	1252.53	1267.46	1189.32
EPA-C15ab	44.95	30.65	1.687	1.1699	1.14	125	142.5	130	1218.02	1111.17	
LKSD1				0.2636	0.32	250	80	94.5	3034.90	3584.98	
LKSD2				0.3517	0.45	250	112.5	109	3198.75	3099.23	

TABLE 5
SUMMARY OF SOIL/MULCH ANALYTICAL RESULTS
SS-17 FULL-SCALE BIOWALL
ALTUS AFB, OKLAHOMA

Sample Identification	Sample Location	Sample Depth (feet bgs) ^{a/}	Sample Date	Sub-Sample	Perrcent Moisture	Percent Solids	Total Iron (1) (mg/kg)	Total Iron (2) (mg/kg)	Total Iron (3) (mg/kg)	Ferrous Iron (4) (mg/kg)	Total Iron (4) (mg/kg)	Freeze CoreWet Sample AVS ^{c/} (mg/kg)	Wet Sample AVS ^{c/} (mg/kg)	Total CRS ^{c/} (mg/kg)	Net CRS (mg/kg)	Sulfur (3) (mg/kg)	Sulfate (5) (mg/kg)
EPA-C11	5 feet east of BB04W	6.0 - 7.5	6-Sep-07	a	33.84	66.16	160	5,283	9,210	1,051	975	321	--	372	--	ND	73
				b	33.83	66.17	166	6,994	12,300	1,275	1,170	380	--	--	--	40	57
				Mean	33.83	66.17	163	6,138	10,755	1,163	1,073	351	--	372	22	40	65
EPA-C13	5 feet east of BB04W	12.0 - 13.5	6-Sep-07	a	38.52	61.48	262	4,142	6,070	830	788	129	--	135	--	42	49
				b	28.53	71.47	285	3,692	--	1,311	1,216	133	--	--	--	--	16
				Mean	33.52	66.48	273	3,917	6,070	1,070	1,002	131	--	135	3.7	42	32
EPA-C13 above 5 feet east of BB04W (replicate)	12.0 - 13.5	6-Sep-07		aa	33.35	66.65	199	5,980	11,300	1,263	1,181	194	--	216	--	ND	32
				bb	19.71	80.29	223	5,271	10,800	1,251	1,197	191	--	--	--	ND	39
				Mean	26.53	73.47	211	5,626	11,050	1,257	1,189	192	--	216	24	ND	36
EPA-C15	5 feet east of BB04W	18.0 - 19.5	6-Sep-07	a	29.72	70.28	285	4,439	8,260	1,031	926	131	--	201	--	127	35
				b	25.28	74.72	237	3,835	--	1,107	1,001	181	--	--	--	--	35
				Mean	27.50	72.50	261	4,137	8,260	1,069	963	156	--	201	45	127	35
EPA-C15 above 5 feet east of BB04W (replicate)	18.0 - 19.5	6-Sep-07		aa	30.65	69.35	147	5,590	8,870	1,253	1,267	220	--	200	--	84	89
				bb	44.95	55.05	158	4,745	--	1,218	1,111	286	--	--	--	--	82
				Mean	30.65	69.35	152	5,168	8,870	1,235	1,189	253	--	200	-53	84	85

NOTE: AVS and CRS extractions were not performed sequentially. Values listed for Net CRS are mean Total CRS values minus mean AVS values.

- (1) Total iron by ICP following extraction with 10 ml ascorbate for 24 hours.
- (2) Total iron by ICP following extraction with 10- ml dithionite extracted for 4 hours at 60 degrees cCelsius.
- (3) Total iron and sulfur by digestion.
- (4) Ferrous and total iron by ICP following extraction with 10 ml 0.5 M HCl for 1 hour.
- (5) Sulfate following extraction with 20 ml 2.4mM NaHCO₃ and 2.6mM Na₂CO₃ for 24 hours.

^{a/} feet bgs = feet below ground surface.

^{b/} mg/kg = micrograms per kilogram dry weight.

^{c/} AVS = acid volatile sulfide; CRS = chromium reducible sulfide.

TABLE 6
SOIL AND MULCH ANALYSIS RESULTS FOR BIOGEOCHEMICAL REDUCTION EVALUATION
SS-17 BIOWALL TECHNICAL SUMMARY REPORT
ALTUS AFB, OKLAHOMA

Sample Identification	Sample Depth (ft bgs) ^{a/}	Sample Date	Acid Volatile Sulfide (mg/kg)	Chromium Extractable Sulfide (mg/kg)	Oxidized Iron (mg/kg dry)	Bioavailable Ferric Iron (mg/kg dry) ^{b/}	Strong Acid Ferric Iron (mg/kg dry)	Strong Acid Soluble Ferrous Iron (mg/kg dry)	Strong Acid Divalent Manganese (mg/kg dry)	Weak Acid Soluble Ferric Iron (mg/kg dry)	Weak Acid Soluble Ferrous Iron (mg/kg dry)	Weak Acid Soluble Divalent Manganese (mg/kg dry)	Percent Solids (percent)
BB04U	10.5 - 11.5'	18-Oct-06	460	800 B ^{c/}	<5.8	<5.8	11,400	1,000	428	<115	<115	140	87
BB04U	25.5 - 26.5'	18-Oct-06	602	700 B	24.3	<5.7	17,400	784	242	<114	<114	<114	88
BB04W ^{d/}	11 - 12'	19-Oct-06	931	1,800 B	<5.8	<5.8	1,920	4,100	<230	<115	477	<115	87
BB04W ^{d/}	25 - 26'	19-Oct-06	<1,149	<1,200	<5.8	<5.8	9,080	5,740	<230	<115	244	<115	87
BB04D	8.5 - 9'	18-Oct-06	454	700 B	<5.8	<5.8	8,610	<233	<233	<116	<116	<116	86
BB04D	26 - 27'	18-Oct-06	575	1,100 B	<5.8	<5.8	26,600	1,220	1,040	<115	<115	136	87
BB05W	11 - 12'	19-Oct-06	<1,149	1,800	<5.8	126	550	2,160	<230	163	779	<115	87
BB05W	25 - 26'	19-Oct-06	<1,136	<1,100	<5.7	493	<227	1,610	<227	<114	407	<114	88
BB05D	25 - 25.5'	19-Oct-06	<1,163	<1,200	30.9	2,430	9,820	<233	<233	<116	<116	<116	86
BC07W	14 - 15'	20-Oct-06	<1,163	<1,200	<5.8	1,940	509	1,720	<233	<116	497	<116	86
BC07W	25.5 - 26'	20-Oct-06	<1,149	<1,200	27	488	<230	1,500	<230	<115	582	<115	87
BC07D	13 - 14'	20-Oct-06	<1,149	<1,200	1,160	73.3	3,170	<230	371	<115	<115	<115	87
BC07D	25 - 26'	20-Oct-06	<1,111	<1,100	<5.6	2,230	8,220	1,440	<222	303	580	<111	90
BF12W	12 - 13'	19-Oct-06	954	900 B	37.8	<5.8	521	1,190	<230	<115	424	<115	87
BF12W	25.5 - 26.5'	19-Oct-06	386	<100	<5.7	<5.7	297	957	<227	<114	307	<114	88
BF12D	9 - 10'	16-Oct-06	494	1,400 B	72.0	<5.8	<230	570	<230	<115	<115	<115	87
BF12D	34 - 35'	16-Oct-06	430	900 B	145.0	<5.8	5,140	990	<233	<116	176	<116	86

^{a/} ft bgs = feet below ground surface.

^{b/} mg/kg dry = milligram per kilogram dry weight.

^{c/} B indicates the analyte was detected in the blank sample.

EPA Column Study (Altus Site SS-17) – No Data

Dover AFB

15ml 0.5M HCl extraction of Dover samples

Sample	location	wet wt (g)	H2O %	dry wt (g)	measured Fe2+ (mg/L)	dilution x250 (mg/L)	Fe2+ (mg/kg)	Fe2+ mean (mg/kg)	stdev
TSB1-10a		1.849	27.54	1.339732	1.06	265	2967.01	3520.40	782.61
TSB1-10b		1.461	27.54	1.058598	1.15	287.5	4073.78		
TSB1-17a		1.947	24.54	1.469209	1.65	412.5	4211.45	4173.48	53.69
TSB1-17b		1.442	24.54	1.088135	1.2	300	4135.52		
TSB3-10a		2.474	29.04	1.755628	1.67	417.5	3567.10	3327.11	339.39
TSB3-10b		1.455	29.04	1.032513	0.85	212.5	3087.13		
TSB3-16a		1.636	29.02	1.161182	0.93	232.5	3003.41	2906.23	137.43
TSB3-16b		1.768	29.02	1.254871	0.94	235	2809.05		
TSB6-10a		2.118	28.12	1.522395	1.41	352.5	3473.15	3589.40	164.42
TSB6-10b		1.788	28.12	1.285195	1.27	317.5	3705.66		
TSB6-17a		1.402	28.99	0.995611	0.72	180	2711.90	2693.01	26.72
TSB6-17b		1.876	28.99	1.332215	0.95	237.5	2674.12		
TSB8-10a		1.84	24.77	1.384241	0.71	177.5	1923.44	1993.97	99.75
TSB8-10b		1.835	24.77	1.380479	0.76	190	2064.50		
TSB8-17a		1.394	24.82	1.048046	0.88	220	3148.72	2964.75	260.17
TSB8-17b		1.704	24.82	1.281112	0.95	237.5	2780.79		
lksd1				0.14	0.12	30	3214.29	3156.73	81.40
lksd2				0.1936	0.16	40	3099.17		
es-sed1				0.1599	0.22	55	5159.47	4891.38	379.14
es-sed2				0.146	0.18	45	4623.29		

Seneca Depot

15ml 0.5M HCl extraction

No.	Sample	location	wet wt (g)	H2O %	dry wt (g)	measured	dilution x250 (mg/L)	Fe2+ (mg/kg)	Fe2+ mean (mg/kg)	stdev
						Fe2+ (mg/L) (mg/L)				
1	Seneca A1a	6.0-8.0	2.74	28.67	1.954394	0.7	175	1343.13	1523.94	255.71
	Seneca A1b		2.498	28.67	1.781779	0.81	202.5	1704.76		
2	Seneca A1	9.0-11.0	2.578	26.12	1.904679	0.85	212.5	1673.51	1838.21	232.92
	Seneca A2		2.078	26.12	1.535269	0.82	205	2002.91		
3	Seneca B1a	7.0-9.0	3.068	24.39	2.319581	0.77	192.5	1244.84	1391.18	206.96
	Seneca B1b		1.742	24.39	1.31705	0.54	135	1537.53		
4	Seneca B1a	9.5-7.5	1.918	29.78	1.34691	0.91	227.5	2533.58	2550.72	24.25
	Seneca B1b		1.83	29.78	1.285112	0.88	220	2567.87		

Dugway PG

15ml 0.5M HCl extraction of Dugway samples

Sample	location	wet wt (g)	H2O %	dry wt (g)	measured	dilution x250 (mg/L)	Fe2+ (mg/kg)	Fe2+ mean (mg/kg)	stdev
					Fe2+ (mg/L)				
FD90a		2.152	16.79	1.79072	0.39	97.5	816.71	829.92	18.69
FD90b		2.138	16.79	1.779071	0.4	100	843.14		
SO86a		2.882	14.08	2.476128	0.06	15	90.87	94.42	5.02
SO86b		2.673	14.08	2.296561	0.06	15	97.97		
SO87a		2.71	14.70	2.311624	0.21	52.5	340.67	337.71	4.19
SO87b		2.364	14.70	2.016487	0.18	45	334.74		
SO88a		2.811	15.49	2.375467	0.54	135	852.46	863.31	15.34
SO88b		2.792	15.49	2.35941	0.55	137.5	874.16		
SO89a		3.025	17.10	2.507769	0.45	112.5	672.91	685.59	17.93
SO89b		2.073	17.10	1.718547	0.32	80	698.26		
SO90a		2.943	18.42	2.400961	0.43	107.5	671.61	663.17	11.93
SO90b		2.738	18.42	2.233718	0.39	97.5	654.74		
SO91a		3.128	12.89	2.724812	0.93	232.5	1279.90	1334.96	77.86
SO91b		2.075	12.89	1.80754	0.67	167.5	1390.01		

Carbon and Moisture Data

CUSTOMER #:
02343

HUFFMAN
LABORATORIES, INC.
Quality Analytical Services Since 1936

4630 Indiana Street • Golden, CO 80403
Phone: (303) 278-4455 • FAX: (303) 278-7012

DATE 2/20/08
LAB# 102108
P.O.
RECD 01/11/08

ANALYSIS REPORT

PAT EVANS
CDM
11811 NE FIRST STREET
BELLEVUE WA 98009

Received

FEB 25 2008

CDM

SEQUENCE/ SAMPLE ID	01 EPA-C1-A	02 EPA-C3-A	03 EPA-C4-A	04 EPA-C5-A
Drying Loss---%	- 26.21- - - -	38.80- - - -	41.33- - - -	43.51
Total Carbon--%	- - 3.96- - - -	8.55- - - -	9.08- - - -	12.04
Tot CO2 as C--%	- - 0.48- - - -	0.38- - - -	0.49- - - -	0.51
Organic C*----%	- - 3.48- - - -	8.17- - - -	8.59- - - -	11.53
Sulfur-----%	- - 0.16- - - -	0.15- - - -	0.21- - - -	0.31
Sulfate Sulfur%	- - 0.05- - - -	0.03- - - -	0.04- - - -	0.07
Pyritic Sulfur%	- - 0.10- - - -	0.11- - - -	0.16- - - -	0.21
Organic Sulfur%	- - 0.01- - - -	0.01- - - -	0.01- - - -	0.03

SEQUENCE/ SAMPLE ID	05 EPA-C6-A	06 EPA-C7-A	07 EPA-C11-A	08 EPA-C13-A
Drying Loss---%	- 42.38- - - -	39.21- - - -	23.62- - - -	23.34
Total Carbon--%	- 10.96- - - -	9.97- - - -	2.49- - - -	3.09
Tot CO2 as C--%	- - 0.44- - - -	0.43- - - -	0.37- - - -	0.28
Organic C*----%	- 10.52- - - -	9.54- - - -	2.12- - - -	2.81
Sulfur-----%	- - 0.15- - - -	0.13- - - -	0.08- - - -	0.04
Sulfate Sulfur%	- - 0.03- - - -	0.03- - - -	0.04- - - -	0.01
Pyritic Sulfur%	- - 0.02- - - -	0.10- - - -	0.03- - - -	0.02
Organic Sulfur%	- - 0.10- - - -	0.01- - - -	0.01- - - -	0.01

SEQUENCE/ SAMPLE ID	09 EPA-C15-A	10 B3 1-1	11 B3 3-1	12 B3 4-1
Drying Loss---%	- 23.13- - - -	31.33- - - -	33.09- - - -	34.21
Total Carbon--%	- - 3.42- - - -	4.45- - - -	6.50- - - -	7.27
Tot CO2 as C--%	- - 0.29- - - -	0.28- - - -	0.32- - - -	0.30
Organic C*----%	- - 3.13- - - -	4.17- - - -	6.18- - - -	6.97
Sulfur-----%	- - 0.05- - - -	0.82- - - -	0.57- - - -	0.84
Sulfate Sulfur%	- - 0.02- - - -	0.14- - - -	0.13- - - -	0.15
Pyritic Sulfur%	- - 0.02- - - -	0.67- - - -	0.44- - - -	0.68
Organic Sulfur%	- - 0.01- - - -	0.01- - - -	0.01- - - -	0.01

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* * (CONT) * *

ANALYSIS REPORT

PAT EVANS
CDM
11811 NE FIRST STREET
BELLEVUE WA 98009

SEQUENCE/ SAMPLE ID	13 B3 5-1	14 B3 7-1	15 B3 8-1	16 B3 9-1
Drying Loss---%	27.71- - - -	32.90- - - -	27.29- - - -	27.68
Total Carbon--%	4.50- - - -	5.88- - - -	4.22- - - -	4.49
Tot CO2 as C--%	0.29- - - -	0.31- - - -	0.33- - - -	0.30
Organic C*----%	4.21- - - -	5.57- - - -	3.89- - - -	4.19
Sulfur-----%	0.65- - - -	0.86- - - -	0.59- - - -	0.98
Sulfate Sulfur%	0.14- - - -	0.14- - - -	0.15- - - -	0.13
Pyritic Sulfur%	0.50- - - -	0.71- - - -	0.43- - - -	0.85
Organic Sulfur%	0.01- - - -	0.01- - - -	0.01- - - -	0.01

Loss on drying was determined in air at 105 degrees C overnight and is reported on an as received sample basis. All other results are reported on a dried sample basis.

After drying, the samples were ground in entirety prior to all other analyses.

*By difference

Organic sulfur is total sulfur remaining in the sample after extraction with HCl and HNO3.

Sulfate sulfur is the total sulfur in the sample minus the total sulfur content of the sample after extraction with HCl.

Pyritic sulfur is the total sulfur in the HCl extracted sample minus the organic sulfur.

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DATE 6/6/08
LAB# 134908
P.O.
RECD 05/08/08

ANALYSIS REPORT

PAT EVANS
CDM
11811 NE FIRST STREET
BELLEVUE WA 98009

Received
JUN 09 2008
CDM

SEQUENCE/ SAMPLE NUMBER	ANALYSIS							
	Drying Loss---%				Total Carbon--% Tot CO2 as C--% Organic C*----%			
01/097SO086 - - - -	17.46	-	-	-	1.01	-	-	-
02/097SO087 - - - -	16.59	-	-	-	1.12	-	-	-
03/097SO088 - - - -	19.20	-	-	-	1.26	-	-	-
04/097SO089 - - - -	18.94	-	-	-	1.04	-	-	-
05/097SO090 - - - -	19.27	-	-	-	1.03	-	-	-
06/097SO091 - - - -	16.38	-	-	-	1.78	-	-	-
07/097FD090 - - - -	20.11	-	-	-	1.05	-	-	-
08/SENECA A1-6-8 -	30.52	-	-	-	10.44	-	-	-
09/SENECA A1-9-11 -	31.89	-	-	-	6.49	-	-	-
10/SENECA B1-7-9 -	29.55	-	-	-	8.08	-	-	-
11/SENECA B1-7.5-9.5	42.36	-	-	-	13.52	-	-	-
12/TSB1-10 - - - -	28.95	-	-	-	4.83	-	-	-
13/TSB1-17 - - - -	29.41	-	-	-	5.93	-	-	-
14/TSB3-10 - - - -	32.39	-	-	-	6.69	-	-	-
15/TSB3-16 - - - -	30.57	-	-	-	5.45	-	-	-
16/TSB6-10 - - - -	27.76	-	-	-	4.83	-	-	-
17/TSB6-17 - - - -	29.75	-	-	-	5.31	-	-	-

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DATE 6/6/08
LAB# 134908
P.O.
RECD 05/08/08
* * (CONT) * *

ANALYSIS REPORT

PAT EVANS
CDM
11811 NE FIRST STREET
BELLEVUE WA 98009

SEQUENCE/ SAMPLE NUMBER	ANALYSIS
	Drying Loss---% Total Carbon--% Tot CO2 as C--% Organic C*----%
18/TSB8-10 - - - -	29.94- - - - - 5.64- - - - - 0.80- - - - - 4.84
19/TSB8-17 - - - -	29.85- - - - - 5.37- - - - - 1.03- - - - - 4.34
20/TSB16-10 - - - -	29.56 - - - - 4.95 - - - - 0.58 - - - - 4.37

Loss on drying was determined in air at 105 degrees C overnight and is reported on an as received sample basis. All other results are reported on a dried sample basis.

After drying, the samples were ground in entirety prior to all other analyses.

*By difference

Appendix B
Groundwater Analysis Raw Data Reports

VOC Data

Altus Sites OU-1 and SS-17

MEMORANDUM (LABORATORY DATA REPORT)

SHAW ENVIRONMENTAL, Inc.

Contract No. 68-C-03-097

In reply refer to: 07-LH-46

To: Mary Sue McNeil
Dennis Miller

From: Lisa Hudson

Lab: GC

Thru: Sujith Kumar
John Cox

Date: 9/19/07

Technical Directive No.: 40A247SF
Task No.: 19421

Originator: Cherri Adair
Copies: John Wilson
Kevin Smith
Rick Wilkin
Yongtian He
Rebecca Foster
Lisa Hudson
John Cox

Project/Sample Site: Altus AFB Biowall
Date Collected: 9/6/07
Date Received: 9/17/07
Date Analyzed: 9/19/07
No. Samples Analyzed: 11

Shaw Sample Set No.: 4067
Sample Matrix: Water
Analysis Type: Dissolved Gas
Sample Preparation: Not applicable

Method(s) Used : RSKSOP-194 Rev 3 Gas Analysis by MTI Gas Chromatograph
RSKSOP-175 Rev 2 Sample Preparation and Calculations for Dissolved Gas
Analysis in Water Samples Using a GC Headspace Equilibration Technique

Comments:

All samples received were analyzed in accordance with the SOPs listed above. The data quality objective (DQO) for the above referenced methods have been met for all blanks, continuing calibration check standards, second source standards, and duplicate samples. This demonstrates the instrument is in control and the data is valid. All calculations were performed as described in the SOPs.

SHAW ENVIRONMENTAL, Inc.
Analytical Service Results Report

Laboratory:

GC

Report Date:

9/19/07

Technical Directive:

40A247SF

Sample Results (1,2)

Analyst:

Lisa Hudson

Method:

RSKSOP-194 & RSKSOP-175

			Analytes	Methane		Ethylene		Ethane		Acetylene	
			Codes	74-82-8		74-85-1		74-84-0		74-86-2	
			Unit	mg/L, in water		mg/L, in water		mg/L, in water		mg/L, in water	
			MDL	0.0001		0.0003		0.0002		0.0020	
			QL	0.0010		0.0027		0.0020		0.0125	
Lab Sample ID	Date Collected	Date Analyzed	Field Sample ID	Data	DF	Data	DF	Data	DF	Data	DF
4067-1	9/6/07	9/19/07	MP1	1.97	1	ND	1	ND	1	ND	1
4067-2	9/6/07	9/19/07	EPAU-MP1	0.118	1	ND	1	ND	1	ND	1
4067-3	9/6/07	9/19/07	MP2	1.68	1	ND	1	ND	1	ND	1
4067-4	9/6/07	9/19/07	MP3	1.14	1	ND	1	ND	1	ND	1
4067-5	9/6/07	9/19/07	MP4	0.826	1	ND	1	ND	1	ND	1
4067-6	9/6/07	9/19/07	BB04U	0.237	1	ND	1	ND	1	ND	1
4067-7	9/6/07	9/19/07	BB04W	2.43	1	ND	1	ND	1	ND	1
4067-8	9/6/07	9/19/07	BB04D	1.05	1	ND	1	ND	1	ND	1
4067-9	9/6/07	9/19/07	BB05U	0.0480	1	ND	1	ND	1	ND	1
4067-10	9/6/07	9/19/07	BB05W	2.12	1	ND	1	ND	1	ND	1
4067-11	9/6/07	9/19/07	BB05D	0.465	1	ND	1	ND	1	ND	1
4067-11 Lab Dup	9/6/07	9/19/07	BB05D	0.466 (RPD=0.215)	1	ND (RPD=NA)	1	ND (RPD=NA)	1	ND (RPD=NA)	1
4067-11 Field Dup	9/6/07	9/19/07	BB05D	0.549	1	ND	1	ND	1	ND	1

Comments:

The data quality objective (DQO) for the precision of laboratory duplicate samples is a relative percent difference (RPD) of ≤ 20 as specified in the SOP. RPDs were met for the duplicate samples in this sample set.

Notes:

1. If the parameter was detected above the quantitation limit (**QL**), the numeric result is reported; **BQL** denotes that the parameter was not detected at or above the quantitation limit; **BQL ()** denotes that the parameter was detected above the method detection limit (**MDL**) but below **QL** and the estimated numeric result is reported in parenthesis; **ND** denotes that the parameter was not detected at all. All the results are corrected with dilution factors (**DF**), if applicable.
2. " - " denotes that the information is not available or the analyte is not analyzed.

SHAW ENVIRONMENTAL, Inc.
Analytical Service Results Report

Laboratory: GC Report Date: 9/19/07

Technical Directive: 40A247SF

Quality Control Data Summary (1)

Analyst: Lisa Hudson

Method: RSKSOP-194 & RSKSOP-175

			Analytes	Methane			Ethylene			Ethane			Acetylene			Methane			Ethylene			Ethane			Acetylene		
			Codes	74-82-8			74-85-1			74-84-0			74-86-2			74-82-8			74-85-1			74-84-0			74-86-2		
			Unit	ppm, v/v in gas			ppm, v/v in gas			ppm, v/v in gas			ppm, v/v in gas			mg/L, in water			mg/L, in water			mg/L, in water			mg/L, in water		
			MDL	1.17			1.13			0.903			1.63			0.0001			0.0003			0.0002			0.0020		
			QL	10.0			10.0			10.0			10.0			0.0010			0.0027			0.0020			0.0125		
Date Analyzed	Additional ID	Date Prepared	QC Sample ID	Data	True Value	% REC	Data	True Value	% REC	Data	True Value	% REC	Data	True Value	% REC	Data	True Value	% REC	Data	True Value	% REC	Data	True Value	% REC	Data	True Value	% REC
9/19/07	MB	9/19/07	Helium Blank	ND	-	-	ND	-	-	ND	-	-	ND	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	CCC	4/13/06	100 ppm CH4	101	100	101	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	CCC	5/8/07	100 ppm C2H4	-	-	-	99.1	100	99.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	CCC	8/12/04	100 ppm C2H6	-	-	-	-	-	-	106	100	106	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	CCC	2/6/07	100 ppm C2H2	-	-	-	-	-	-	-	-	-	99.3	100	99.3	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	SS	4/13/06	100 ppm CH4	101	100	101	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	SS	4/13/06	100 ppm C2H4	-	-	-	99.9	100	99.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	SS	6/14/04	100 ppm C2H6	-	-	-	-	-	-	107	100	107	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	SS	2/6/07	100 ppm C2H2	-	-	-	-	-	-	-	-	-	99.8	100	99.8	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	MB	9/19/07	Helium Blank	ND	-	-	ND	-	-	ND	-	-	ND	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	CCC	5/8/07	10 ppm C2H4	-	-	-	11.0	10.0	110	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	CCC	2/8/07	10 ppm C2H6	-	-	-	-	-	-	9.69	10.0	96.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	CCC	2/6/07	10 ppm C2H2	-	-	-	-	-	-	-	-	-	10.5	10.0	105	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	CCC	12/13/05	1000 ppm CH4	1020	1000	102	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9/19/07	CCC	12/13/05	100000 ppm CH4	98000	100000	98.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
-	MC	-	Macro Check	-	-	-	-	-	-	-	-	-	-	-	-	0.0010	-	-	0.0027	-	-	0.0020	-	-	0.0125	-	-
9/19/07	MB	9/19/07	H2O Blank	-	-	-	-	-	-	-	-	-	-	-	-	ND	-	-	ND	-	-	ND	-	-	ND	-	-

Comments:
The data quality objective (DQO) for the cleanliness of the helium Method Blank (MB) is that no analytes should be detected. The DQO for the cleanliness of the water MB is that any detected target gases should be <10ppmv. The DQO for the accuracy of the CCCs and second source QC standards is 85-115% recovery. These DQOs were met for the QC samples in this sample set. The macro check (MC) was conducted at the concentration of the quantitation limit.

Notes:
1. **MB** - Method Blank. **CCC** - Continuing Calibration Check. A calibration standard analyzed within the batch of samples. **LCS** - Laboratory Control Spike. A laboratory blank spiked with analytes at known concentrations. **MS** - Matrix Spike. A field sample spiked with known concentrations of analytes. The field sample id is identified. **QC** - Samples obtained from the second sources are identified by their designated names. **DUP** - Field sample duplicate analysis. A sample selected by the lab analyst to analyze as a duplicate. It is reported in the sample result section. **% REC** - Percent Recovery. Calculated as the percentage of the results to the true values. It equals to % accuracy for CCC.

TABLE 2
CHLORINATED ALIPHATIC HYDROCARBONS IN GROUNDWATER
OU-1 BIOWALL DEMONSTRATION
ALTUS AFB, OKLAHOMA

Sample Identification	Sampling Location	Sample Date	PCE ^{a/} (µg/L) ^{b/}	TCE ^{a/} (µg/L)	1,1-DCE ^{a/} (µg/L)	<i>cis</i> -1,2-DCE (µg/L)	<i>trans</i> -1,2-DCE (µg/L)	VC ^{a/} (µg/L)	1,1-DCA ^{a/} (µg/L)	Chloroform (µg/L)
EPAUMP1	30' Upgradient	6-Sep-07	BQL (0.36) ^{c/}	550	BQL (0.34)	91.8	3.47	7.70	<0.5	BQL (0.33)
PES-MP01	Within Biowall	6-Sep-07	<0.5	BQL (0.21)	<0.5	5.27	9.49	53.4	<0.5	<0.5
PES-MP02	5' Downgradient	6-Sep-07	<0.5	1.23	<0.5	15.2	5.22	136	<0.5	<0.5
PES-MP03	10' Downgradient	6-Sep-07	<0.5	15.5	BQL (0.32)	158	12.2	259	<0.5	<0.5
PES-MP04	30' Downgradient	6-Sep-07	<0.5	58.4	0.59	186	31.1	82.6	<0.5	<0.5

^{a/} PCE = tetrachloroethene, TCE = trichloroethene, DCE = dichloroethene, VC = vinyl chloride, DCA = dichloroethane

^{b/} µg/L = micrograms per liter.

^{c/} BQL indicates the concentration is below the quantification limit but above the method detection limit; the concentration is estimated.

EPA Column Study (Altus SS-17)

Analysis result of column B3 influent (supply bag) and effluent (B3E)
Column B3E sampled 5/15/07

Parameters	Column B3E	Supply bag	Unit
Temp	22.3		C
Conductivity	5892		uS
DO	4.11		mg/L
pH	7.35		
ORP	-105.7		mv
S ²⁻	7.55	0	mg/L
Fe ²⁺	0.04	0	mg/L
TOC	5.39	0.85	mg/L
TC	209	49.1	mg/L
TIC	204	48.3	mg/L
Cl ⁻	812	822	mg/L
SO ₄ ²⁻	1670	2440	mg/L
vinyl chloride	1.59	ND	µg/L
1,1-dichloroethene	1.19	ND	µg/L
methylene chloride	ND	ND	µg/L
trans-1,2-dichloroethene	ND	ND	µg/L
1,1-dichloroethane	ND	ND	µg/L
cis-1,2-dichloroethene	13.5	ND	µg/L
chloroform	ND	ND	µg/L
1,1,1-trichloroethane	ND	ND	µg/L
carbon tetrachloride	ND	ND	µg/L
1,2-dichloroethane	ND	8.5	µg/L
trichloroethene	17.2	2585*	µg/L
Ag	ND	ND	mg/L
Al	0.154	0.345	mg/L
As	0.039	0.035	mg/L
B	5.26	3.95	mg/L
Ba	0.161	0.012	mg/L
Be	BQL(0.001)	ND	mg/L
Ca	436	506	mg/L
Cd	ND	ND	mg/L
Co	BQL(0.002)	ND	mg/L
Cr	BQL(0.002)	0.007	mg/L
Cu	ND	BQL(0.010)	mg/L
Fe	ND	0.067	mg/L
K	9.31	8.81	mg/L
Mg	183	189	mg/L
Mn	BQL(0.003)	ND	mg/L
Mo	BQL(0.001)	0.011	mg/L
Na	790	815	mg/L
Ni	ND	0.054	mg/L
Pb	ND	ND	mg/L
Sb	0.015	0.019	mg/L
Se	BQL(0.008)	0.020	mg/L
Sr	7.71	7.93	mg/L
Ti	0.007	0.015	mg/L
Tl	0.039	0.042	mg/L
V	ND	0.007	mg/L
Zn	0.050	0.341	mg/L

Column Study Analytical Results																					
Sample Identification	Sample Label	Sample Date	Time Days	MW				Cl ⁻ mg/L	SO ₄ ²⁻ mg/L	N (nitrate+nitrite) mg/L nd<1.2	TOC mg/L	DC mg/L	DOC mg/L	DIC mg/L	56.00 32.00		Temp °C	Conductivity µs/cm	DO mg/L	pH	ORP mV
				Methane mg/L	Ethylene mg/L	Ethane mg/L	Acetylene mg/L								Fe ²⁺ mg/L	S ²⁻ mg/L					
		5/15/2007						822	2440	NO SAMPLE	0.85	49		48							
B3 Effluent	B3E	10/18/2004	1	0.242	ND	ND	ND	872	935	ND	1439.74		1340.00		9.75	0.13	22.1	4543	0.23	6.55	-280
		11/15/2004	29	4.310	ND	ND	ND	783	582	ND	139.40		112.82		0.80	0.79	22.7	4061	0.30	6.73	-258
		12/22/2004	66	2.500	ND	ND	ND	723	368	ND	49.80		42.30		0.45	8.50	22.6	3375	0.10	6.64	-313
		1/24/2005	99	4.880	ND	ND	ND	752	595	ND	33.17		26.72		0.10	15.00	23.2	4099	0.08	6.68	-275
		2/22/2005	128	6.410	ND	ND	ND	679	588	0.75	169.25		165.81		0.25	7.25	21.9	3248	0.05	6.85	-233
		3/23/2005	157	3.960	ND	ND	ND	709	835	ND	19.15		14.70		0.15	7.25	23.0	2524	0.05	7.01	-246
		4/22/2005	187	3.370	ND	ND	ND	652	709	ND	19.00		15.80		0.20	4.10	22.6	3350	0.04	7.08	-275
		5/23/2005	218	2.990	ND	ND	ND	661	699	ND	12.90		11.20		0.00	4.40	22.9	2856	0.04	7.14	-274
		6/23/2005	249	6.700	ND	ND	ND	707	773	0.58	17.50		12.50		0.00	6.40	22.7	3120	0.19	7.19	-291
		9/2/2005	320	6.270	ND	ND	ND	750	612	ND	17.29		14.51		0.00	11.75	22.5	4694	0.09	7.29	-370
		11/4/2005	383	3.540	ND	ND	ND	780	1110	ND	11.77		10.04		0.00	15.25	22.8	5184			
		1/29/2006	469																		
		3/1/2006	500										10.50						7.07	-276	
		5/18/2006	578										28.70					3.39	6.95	-175	
		6/26/2006	617								9.43		8.05		0.10	0.00	15.9	6922	1.28	7.30	-240
		7/24/2006	645	1.310	ND	ND	ND				8.57		7.18		0.00	1.37	22.5	5374	1.20	7.27	-275
		8/21/2006	673	0.795	ND	ND	ND	666	1320	ND	7.25		6.71		0.05	11.25	22.2	5637	1.30	7.42	-252
		9/18/2006	701	1.370	ND	ND	ND	680	1510	ND	6.95		5.98		0.00	11.00	21.1	5716	2.62	7.34	-214
		10/24/2006	737	1.93	ND	ND	ND								0.00	7.75	21.7	6191	2.41	7.27	-261.50
		11/20/2006	764					706	1500	ND	6.88		6.55		0.00	4.50	21.9	6428	3.15	7.05	198
		12/19/2006	793					709	1450	ND	7.86		6.05		0.00	9.75	21.5	6532	1.71	7.34	-213
		2/21/2007	857					721	1690	ND	6.00	215	5.31	210	0.00	16.00	21.9	5854	1.42	6.76	-174
		4/23/2007	918					750	1600	ND											
		5/15/2007	940					812	1670	NO SAMPLE	5.39	209		204							

Dover AFB

TABLE 5
SUMMARY OF CHLORINATED ALIPHATIC HYDROCARBONS IN GROUNDWATER
SITE WP-14 BIOWALL PILOT TEST, DOVER AFB, DELAWARE

Sample Location	Location S Description	ample Date	PCE ^{a/} (µg/L) ^{b/}	TCE ^{a/} (µg/L)	1,1-DCE ^{a/} (µg/L)	cis -1,2-DCE (µg/L)	trans -1,2-DCE (µg/L)	VC ^{a/} (µg/L)	1,1-DCA ^{a/} (µg/L)	1,2-DCA (µg/L)	1,1,2-TCA (µg/L)	Chloroethane (µg/L)	Carbon Disulfide (µg/L)	2-Butanone (µg/L)	Acetone (µg/L)
Common Background Monitoring Well															
GSCP9A	25 feet upgradient	1/19/2005	2,039	509	<2.2	752	<3.9	11.6J ^{c/}	<2.2	<1.8	<4.3	<8.3	NA	<68	<23
		2/16/2005	2,546	574	<2.2	868	<3.9	<3.1	<2.2	<1.8	<4.3	<8.3	NA	<68	<23
		3/30/2005	3,850	777	<2.2	1,180	<3.9	<3.1	<2.2	<1.8	<4.3	<8.3	NA	<68	<23
		5/25/2005	4,484	855	<4.4	1,019	<7.8	<6.2	<4.4	<3.6	<8.6	<16.6	NA	<136	<46
		7/20/2005	3,880	710	<2.2	1,010	<3.9	<3.1	<2.2	<1.8	<4.3	<8.3	NA	<68	<23
		12/9/2005	396	80.8	<0.55	156	<0.98	<0.78	<0.55	<0.45	<1.2	<2.1	NA	<17	<5.8
		6/8/2006	1,300	230	<1.0	370	1.3	0.73	<1.0	<1.0	<1.0	<1.0	NA	<10	<10
		3/27/2007	496	80	ND ^{d/}	199	ND	5.75	ND	ND	ND	ND	NA	ND	ND
North Transect Monitoring Wells															
TS-MW11	5 feet upgradient east transect	12/12/2004	40.9	7.12	<0.04	8.87	<0.08	<0.06	<0.04	0.92J	<0.09	<0.17	NA	<1.36	<0.46
		1/18/2005	48.9	8.51	<0.04	14.4	<0.08	0.22J	<0.04	2.20	<0.09	<0.17	NA	<1.36	<0.46
		2/10/2005	49.0	8.28	<0.04	9.44	<0.08	<0.06	<0.04	1.11	<0.09	<0.17	NA	<1.36	<0.46
		3/30/2005	65.5	9.99	<0.04	14.9	<0.08	<0.06	<0.04	1.77	<0.09	<0.17	NA	<1.36	<0.46
		5/25/2005	62.6	10.6	<0.04	18.8	<0.08	0.28J	<0.04	3.11	<0.09	<0.17	NA	<1.36	<0.46
		7/20/2005	61.0	10.6	<0.04	18.2	<0.08	0.30J	<0.04	2.88	<0.09	<0.17	NA	<1.36	<0.46
		12/9/2005	38.1	8.94	<0.04	15.6	<0.08	0.46J	<0.04	2.92	<0.09	<0.17	NA	<1.36	<0.46
		3/18/2008	11.0	1.70	<1.00	3.10	<1.00	<1.00	<1.00	<1.00	<1.00	<1.00	<1.00	<2.00	<5.00
	(duplicate)	3/18/2008	11.0	1.60	<1.00	3.20	<1.00	<1.00	0.37 J	<1.00	<1.00	<1.00	<1.00	<2.00	<5.00
	TS-MW01	in upgradient wall north transect	12/12/2004	13.5	2.60	<0.02	2.66	<0.04	<0.03	<0.02	0.19J	<0.04	<0.08	NA	1.50J
1/18/2005			11.0	2.48	<0.02	6.79	<0.04	<0.03	<0.02	0.28J	<0.04	<0.08	NA	5.40J	62.2
2/10/2005			9.65	2.45	<0.02	21.0	<0.04	<0.03	<0.02	0.32J	<0.04	<0.08	NA	3.40J	26.3
3/30/2005			10.6	2.13	<0.02	32.7	<0.04	<0.03	<0.02	<0.03	<0.04	<0.08	NA	3.90J	19.9
5/25/2005			10.3	2.23	<0.02	34.7	<0.04	<0.03	<0.02	0.80	<0.04	<1.00	NA	6.00J	20.7
7/19/2005			17.1	3.65	<0.02	47.7	0.12 J	0.22 J	<0.02	1.32	<0.04	<0.08	NA	<0.68	13.9
12/8/2005			12.6	3.98	<0.02	33.0	<0.04	0.25 J	<0.02	1.86	<0.04	<0.08	NA	<0.68	0.23
3/19/2008			17.0	3.80	<1.0	23.0	<1.0	0.64 J	<1.0	0.96 J	<1.0	<1.0	<1.0	2.1	1.5 J
TS-MW02	between walls north transect	12/14/2005	30.9	6.10	<0.02	9.44	<0.04	0.15J	<0.02	1.46	1.09	<0.08	NA	<0.68	<0.23
		1/18/2005	25.9	5.77	<0.02	10.5	<0.04	<0.03	<0.02	2.37	<0.04	<0.08	NA	<0.68	<0.23
		2/10/2005	30.6	6.50	<0.02	11.2	<0.04	0.18J	<0.02	2.51	<0.04	<0.08	NA	<0.68	<0.23
		3/30/2005	30.2	6.25	<0.02	11.4	<0.04	0.15J	<0.02	2.73	<0.04	<0.08	NA	<0.68	<0.23
		5/25/2005	21.4	4.74	<0.02	7.98	<0.20	<0.03	<0.02	2.14	<0.04	<0.08	NA	<0.68	<0.23
		7/20/2005	29.5	5.79	<0.02	7.63	<0.04	<0.03	<0.02	1.48	<0.04	<0.08	NA	<0.68	1.52
		12/9/2005	18.1	4.78	<0.02	9.92	<0.04	<0.03	<0.02	1.23	<0.04	<0.08	NA	<0.68	<0.23
		3/19/2008	5.1	1.70	<1.00	9.60	<1.00	1.70	<1.00	1.20	0.90 J	<1.00	<1.00	<2.00	1.20 J
TS-MW03	in down gradient wall north transect	12/12/2004	7.89	1.78	<0.02	2.90	<0.04	<0.03	<0.02	0.32J	<0.04	<0.08	NA	1.90J	30.6
		1/18/2005	2.12	0.6J	<0.02	3.01	<0.04	<0.03	<0.02	0.19J	<0.04	<0.08	NA	48.8	134
		2/15/2005	3.28	0.87J	<0.02	4.96	<0.04	<0.03	<0.02	0.17J	<0.04	<0.08	NA	24.8	60.3
		3/30/2005	3.84	1.01	<0.02	11.6	<0.04	<0.03	<0.02	0.30J	<0.04	<0.08	NA	41.9	76.1
		5/24/2005	6.75	2.40	<0.04	21.6	<0.08	<0.06	<0.04	1.23	<0.09	<0.17	NA	41.5	73.2
		7/20/2005	5.93	1.89	<0.02	19.3	<0.04	0.26J	<0.02	1.47	<0.04	<0.08	NA	45.7	58.0
		12/8/2005	4.99	1.96	<0.02	20.5	0.11J	0.43J	<0.02	1.43	<0.04	<0.08	NA	1.01J	10.8
		3/19/2008	18.00	3.10	<1.0	7.90	<1.00	<1.00	<1.00	0.69 J	<1.00	<1.00	<1.00	<2.00	<5.00
TS-MW04	15 feet down gradient north transect	12/12/2004	32.6	6.53	<0.02	14.3	<0.04	0.28J	<0.02	2.80	<0.04	<0.08	NA	<0.68	<0.23
		1/19/2005	13.4	2.74	<0.02	4.92	<0.04	<0.03	<0.02	0.82	<0.04	<0.08	NA	<0.68	<0.23
		2/10/2005	8.78	1.72	<0.02	2.64	<0.04	<0.03	<0.02	0.39J	<0.04	<0.08	NA	<0.68	<0.23
		3/29/2005	1.84	0.41J	<0.02	0.56J	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		5/24/2005	2.11	0.54J	<0.02	2.08	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		7/19/2005	0.95J	0.20J	<0.02	0.44J	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	1.43J
		12/8/2005	3.58	0.87J	<0.02	1.87	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		3/19/2008	46.0	12.0	<1.00	19.0	<1.00	12.0	<1.00	<1.00	<1.00	<1.00	<1.00	<2.00	<5.00
TS-MW05	30 feet down gradient north transect	12/15/2004	24.1	4.49	<0.02	5.04	<0.04	<0.03	<0.02	0.17J	<0.04	<0.08	NA	<0.68	<0.23
		1/19/2005	43.1	7.02	<0.02	8.40	<0.04	<0.03	<0.02	0.55	<0.04	<0.08	NA	<0.68	<0.23
		2/10/2005	52.1	9.78	<0.02	10.0	<0.04	<0.03	<0.02	0.67	<0.04	<0.10	NA	<0.68	<0.23
		3/29/2005	52.6	11.3	<0.02	11.9	<0.04	<0.03	<0.02	0.73	<0.04	<0.08	NA	<0.68	<0.23
		5/24/2005	45.8	9.55	<0.02	14.4	<0.04	0.17J	<0.02	1.11	<0.04	<0.08	NA	<0.68	<0.23
		7/19/2005	25.5	5.47	<0.02	23.0	<0.04	0.20J	<0.02	0.90	<0.04	<0.08	NA	<0.68	1.34J
		12/7/2005	9.40	2.34	<0.02	9.24	<0.04	<0.03	<0.02	0.44J	<0.04	<0.08	NA	<0.68	<0.23

<div>TABLE 5</div> <div>SUMMARY OF CHLORINATED ALIPHATIC HYDROCARBONS IN GROUNDWATER</div> <div>SITE WP-14 BIOWALL PILOT TEST, DOVER AFB, DELAWARE</div>															
Sample	Location S	ample	PCE ^{a/}	TCE ^{a/}	1,1-DCE ^{a/}	<i>cis</i> -1,2-DCE	<i>trans</i> -1,2-DCE	VC ^{a/}	1,1-DCA ^{a/}	1,2-DCA	1,1,2-TCA	Chloroethane	Carbon Disulfide	2-Butanone	Acetone
Location	Description	Date	(µg/L) ^{b/}	(µg/L)	(µg/L)	(µg/L)	(µg/L)	(µg/L)	(µg/L)	(µg/L)	(µg/L)	(µg/L)	(µg/L)	(µg/L)	(µg/L)
South Transect Monitoring Wells (Amended with Sulfate)															
TS-MW12 duplicate	10 feet upgradient	12/15/2004	0.38J	<0.03	<0.02	0.14J	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
	south transect	12/15/2004	0.36J	<0.03	<0.02	0.12J	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		1/19/2005	1.60	0.33J	<0.02	0.52	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		2/15/2005	11.6	3.44	<0.02	6.77	<0.04	<0.03	<0.02	<0.02	<0.04	6.77	NA	<0.68	<0.23
		3/29/2005	26.6	5.30	<0.02	8.28	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		5/24/2005	24.2	4.92	<0.02	6.94	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		7/18/2005	24.9	4.72	<0.02	6.66	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		12/6/2005	11.8	2.64	<0.02	5.02	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		3/18/2008	2.4	0.29 J	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<2.0	<5.0
TS-MW06	in upgradient wall	12/15/2004	93.6	23.3	<0.09	36.4	<0.16	<0.12	<0.09	<0.07	<0.17	<0.33	NA	<2.72	16.0J
	south transect	1/20/2005	172	37.2	<0.09	114	<0.16	<0.12	<0.09	<0.07	<0.17	<0.33	NA	<2.72	11.3J
		2/15/2005	113	21.8	<0.09	103	<0.16	<0.12	<0.09	<0.07	<0.17	<0.33	NA	<2.72	<0.92
		3/29/2005	109	19.4	<0.11	52.3	<0.20	<0.16	<0.11	<0.09	<0.22	<0.42	NA	<3.41	<1.15
		5/24/2005	55.6	10.5	<0.11	32.6	<0.20	<0.16	<0.11	<0.09	<0.22	<0.42	NA	<3.41	<1.15
		7/19/2005	42.2	7.72	<0.09	23.8	<0.16	<0.12	<0.09	<0.07	<0.17	<0.33	NA	<2.72	4.00J
		12/7/2005	19.1	4.12	<0.02	18.7	0.10J	0.24J	<0.02	<0.02	<0.04	<0.08	NA	<0.68	1.77J
		3/18/2005	2.8	0.93 J	<1.0	1.60	<1.0	0.88 J	<1.0	<1.0	<1.0	<1.0	0.36 J	<2.0	<5.0
TS-MW07	between walls	12/15/2004	29.9	8.58	<0.02	16.4	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
	south transect	1/20/2005	51.2	14.0	<0.02	27.8	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		2/15/2005	25.2	7.37	<0.02	13.4	0.11J	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		3/29/2005	10.0	2.20	<0.02	3.01	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		5/23/2005	17.2	4.17	<0.02	7.32	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		7/19/2005	22.0	5.33	<0.02	11.6	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	1.13J
		12/7/2005	59.2	13.6	<0.02	90.2	0.27J	0.27J	<0.02	<0.02	<0.04	<0.08	NA	<0.68	1.38J
		3/20/2008	11.0	9.8	<1.0	86.0	0.94J	80.0	<1.0	<1.0	<1.0	<1.0	51.00	<2.0	11.0
TS-MW08	in down gradient wall	12/16/2004	38.6	8.95	<0.04	12.0	<0.08	<0.06	<0.04	<0.04	<0.09	<0.17	NA	<1.36	18.9J
	south transect	1/20/2005	4.45	1.48J	<0.04	61.3	0.20J	<0.06	<0.04	<0.04	<0.09	<0.17	NA	16.3J	118
		2/15/2005	9.95	3.55	<0.04	38.8	<0.08	<0.06	<0.04	<0.04	<0.09	<0.17	NA	9.6J	42.0
		3/29/2005	5.46	1.53J	<0.04	28.3	<0.08	<0.06	<0.04	<0.04	<0.09	<0.17	NA	<1.36	<0.46
		5/23/2005	5.30	1.85J	<0.04	65.2	0.31J	<0.06	<0.04	<0.04	<0.09	<0.17	NA	<1.36	3.80J
		7/18/2005	7.44	2.26	<0.04	83.5J	0.56J	0.32J	<0.04	<0.04	<0.09	<0.17	NA	<1.36	5.56J
		12/8/2005	7.56	2.74J	<0.04	85.0	0.70J	1.10J	<0.04	<0.04	<0.09	<0.17	NA	<1.36	4.32J
		3/20/2008	11.0	10.0	<1.0	94.0	1.1	82	<1.0	<1.0	<1.0	<1.0	3.80	<2.0	12.0
TS-MW09	15 feet down gradient	12/16/2004	78.2	15.1	<0.06	18.5	<0.10	<0.08	<0.06	<0.05	<0.11	<0.21	NA	<1.70	<0.58
	south transect	1/20/2005	20.6	4.12	<0.02	5.60	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		2/16/2005	34.4	5.03	<0.02	5.38	0.19J	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		3/28/2005	25.9	4.64	<0.02	6.43	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		5/23/2005	29.0	5.07	<0.02	7.69	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	<0.23
		7/18/2005	51.4	8.53	<0.02	15.0	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	1.01
		12/6/2005	31.1	4.58	<0.02	11.8	<0.04	<0.03	<0.02	<0.02	<0.04	<0.08	NA	<0.68	1.20J
		3/17/2008	37.0	4.50	<1.0	7.9	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<1.0	<2.0	<5.0
TS-MW10	25 feet down gradient	12/16/2004	51.4	7.60	<0.04	6.65	<0.08	<0.06	<0.04	<0.04	<0.09	<0.17	NA	<1.36	<0.46
	south transect	1/19/2005	185	42.4	<0.02	63.4	<0.08	0.6J	<0.02	<0.02	<0.09	<0.17	NA	<1.36	<0.46
		2/16/2005	384	96.6	<0.04	145	<0.98	<0.78	<0.04	<0.04	<0.09	<0.17	NA	<1.36	<0.46
		3/28/2005	501	90.0	<0.55	118	<0.98	<0.78	<0.55	<0.45	<1.08	<2.08	NA	<17.0	<5.75
		5/23/2005	1,100	336	<0.55	481	<0.98	11.0J	<0.55	<0.45	<1.08	<2.08	NA	<17.0	<5.75
		7/18/2005	682	226	<0.55	280	<0.98	5.75J	<0.55	<0.45	<1.08	<2.08	NA	<17.0	23.2
		12/6/2005	38.1	8.94	<0.04	15.6	<0.08	0.46J	<0.04	2.92	<0.09	<0.17	NA	<1.36	<0.46

^{a/} PCE = tetrachloroethene, TCE = trichloroethene, DCE = dichloroethene, VC = vinyl chloride, and DCA = dichloroethane.

^{b/} µg/L = micrograms per liter.

^{c/} J-flag indicates the concentration is estimated.

^{d/} ND indicates the analyte was not detected.

TABLE 3
SUMMARY OF CHLORINATED ALIPHATIC HYDROCARBONS IN GROUNDWATER
SITE WP-14 BIOWALL PILOT TEST, DOVER AFB, DELAWARE

Sample Location	Location Sa Description	mple Date	PCE ^{a/} (µg/L) ^{b/}	TCE ^{a/} (µg/L)	1,1-DCE ^{a/} (µg/L)	cis -1,2-DCE (µg/L)	trans -1,2-DCE (µg/L)	VC ^{a/} (µg/L)	1,1-DCA ^{a/} (µg/L)	1,2-DCA (µg/L)	1,1,2-TCA (µg/L)	Chloroethane (µg/L)	Carbon Disulfide (µg/L)	2-Butanone (µg/L)	Acetone (µg/L)	Isopropylbenzene (µg/L)	Benzene (µg/L)	Toluene (µg/L)
North Transect Monitoring Wells																		
TS-MW11 (duplicate)	5' Upgradient of East Biowall	3/18/2008	11.0	1.70	<1.00	3.10	<1.00	<1.00	<1.00	<1.00	<1.00	<1.00	<1.00	<2.00	<5.00	<1.00	<1.00	<1.00
		3/18/2008	11.0	1.60	<1.00	3.20	<1.00	<1.00	0.37 J	<1.00	<1.00	<1.00	<1.00	<2.00	<5.00	0.91 J	0.29 J	<1.00
TS-MW01	Within First (East) Biowall	3/19/2008	17.0	3.80	<1.00	23.0	<1.00	0.64 J	<1.00	0.96 J	<1.00	<1.00	<1.00	2.10	1.5 J	2.20	0.74 J	<1.00
TS-MW02	Between Biowalls	3/19/2008	5.1	1.70	<1.00	9.60	<1.00	1.70	<1.00	1.20	0.90 J	<1.00	<1.00	<2.00	1.20 J	1.30	0.83 J	<1.00
TS-MW03	Within Second (West) Biowall	3/19/2008	18.0	3.10	<1.00	7.90	<1.00	<1.00	<1.00	0.69 J	<1.00	<1.00	<1.00	<2.00	<5.00	0.46 J	0.68 J	<1.00
TS-MW04	15' Downgradient of West Biowall	3/19/2008	46.0	12.0	<1.00	19.0	<1.00	12.0	<1.00	<1.00	<1.00	<1.00	<1.00	<2.00	<5.00	<1.00	<1.00	<1.00
South Transect Monitoring Wells (Amended with Sulfate)																		
TS-MW12	10' Upgradient of East Biowall	3/18/2008	2.40	0.29 J	<1.00	<1.00	<1.00	<1.00	<1.00	<1.00	<1.00	<1.00	<1.00	<2.00	<5.00	<1.00	<1.00	<1.00
TS-MW06	Within First (East) Biowall	3/18/2005	2.80	0.93 J	<1.00	1.60	<1.00	0.88 J	<1.00	<1.00	<1.00	<1.00	0.36 J	<2.00	<5.00	<1.00	<1.00	<1.00
TS-MW07	Between Biowalls	3/20/2008	11.0	9.80	<1.00	86.0	0.94J	80.0	<1.00	<1.00	<1.00	<1.00	51.0	<2.00	11.0	<1.00	<1.00	<1.00
TS-MW08	Within Second (West) Biowall	3/20/2008	11.0	10.0	<1.00	94.0	1.10	82.0	<1.00	<1.00	<1.00	<1.00	3.80	<2.00	12.0	<1.00	<1.00	0.61J
TS-MW09	15' Downgradient of West Biowall	3/17/2008	37.0	4.50	<1.00	7.90	<1.00	<1.00	<1.00	<1.00	<1.00	<1.00	<1.00	<2.00	<5.00	<1.00	<1.00	<1.00

^{a/} PCE = tetrachloroethene, TCE = trichloroethene, DCE = dichloroethene, VC = vinyl chloride, and DCA = dichloroethane.

^{b/} µg/L = micrograms per liter.

^{c/} J-flag indicates the concentration is estimated.

^{d/} ND indicates the analyte was not detected.

Seneca Depot

TABLE 3
SUMMARY OF VOLATILE ORGANIC COMPOUNDS IN GROUNDWATER
ASH LANDFILL BIOWALL, SENECA ARMY DEPOT ACTIVITY, NEW YORK

Sample Identification	Location Description	Sample Date	PCE ^{a/} (µg/L) ^{b/}	TCE µg/L	1,1-DCE µg/L	<i>cis</i> -1,2-DCE µg/L	<i>trans</i> -1,2-DCE µg/L	VC µg/L	1,1-DCA µg/L
PT-18A	Upgradient of Biowall A	15-Nov-07	<1.0	2,700	2.1	720	3.4	8.2	<1.0
MWT-25	Upgradient of Biowall A	15-Nov-07	<1.0	26	<1.0	17	<1.0	0.64 J ^{c/}	<1.0
TEMP-1	In Biowall A	10-Jan-08	<1.0	3.6	<1.0	53	1.5	24	<1.0
MWT-26	Upgradient of Biowalls B1/B2	15-Nov-07	<1.0	2.8	<1.0	2.8	<1.0	<1.0	<1.0
MWT-27	Within Biowall B1	15-Nov-07	<10	<10	<10	<10	<10	<10	<10
MWT-28	Within Biowall B2	15-Nov-07	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0	<5.0
MWT-29	Downgradient of Biowall B2	14-Nov-07	<1.0	4.4	<1.0	96	0.83 J ^{c/}	74	<1.0
MWT-22	Downgradient of Biowall B2	14-Nov-07	<1.0	2.6	<1.0	99	0.85 J	180	<1.0
PT-22	Between Biowalls B and C	14-Nov-07	<1.0	9.7	<1.0	30	0.67 J	11	<1.0
MWT-23	Within Biowall C2	16-Nov-07	<7.0	<7.0	2.55 J	3.55 J	<7.0	3.65 J	<7.0
MWT-24	Downgradient of Biowalls C1/C2	13-Nov-07	<1.0	1.6	<1.0	6.7	<1.0	3.8	<1.0
PT-17	Downgradient of Biowalls C1/C2	13-Nov-07	<1.0	15	<1.0	27	0.54 J	22	<1.0
MWT-7	Upgradient of ZVI wall	13-Nov-07	<1.0	510	<1.0	90	<1.0	24	<1.0
PT-24	Downgradient of ZVI wall	13-Nov-07	<1.0	3.8	<1.0	39	<1.0	<1.0	0.56 J

^{a/} PCE = tetrachloroethene, TCE = trichloroethene, DCE = dichloroethene, VC = vinyl chloride, DCA = dichloroethane.

^{b/} µg/L = micrograms per liter.

^{c/} J-flag indicates the concentration is below the quantification limit but above the method detection limit, and the concentration is estimated.

Dugway PG

TABLE 3
CHLORINATED ALIPHATIC HYDROCARBONS IN GROUNDWATER
SWMU-97 PILOT TEST, DUGWAY PROVING GROUND, UTAH

Sample Identification	Sample Date	PCE ^{a/} (µg/L) ^{b/}	TCE ^{a/} (µg/L)	1,1-DCE ^{a/} (µg/L)	<i>cis</i> -1,2-DCE (µg/L)	<i>trans</i> -1,2-DCE (µg/L)	VC ^{a/} (µg/L)	Chloroform (µg/L)	Methylene Chloride (µg/L)
TW22	24-Apr-08	18 J ^{c/}	2,300	<50	6.1 J	<50	<50	7.7 J	<50
Duplicate	24-Apr-08	12 J	1,300	<50	<50	<50	<50	<50	<50
TW23	24-Apr-08	<50	660	<50	<50	<50	<50	<50	<50
TW24	22-Apr-08	11 J	1,300	<20	<20	<20	<20	6.2 J	<20
TW25	23-Apr-08	12 J	1,400	<50	<50	<50	<50	8.6 J	<50
TW26	23-Apr-08	23 J	2,500	<100	<100	<100	<100	12 J	<100
TW27	23-Apr-08	<100	790	<100	<100	<100	<100	<100	<100
TW28	23-Apr-08	<100	1,500	<100	<100	<100	<100	<100	<100
TW29	23-Apr-08	10 J	1,800	<50	<50	<50	<50	<50	<50
IW02	24-Apr-08	41 J	<50	<50	<50	<50	<50	<50	<50
IW03	24-Apr-08	10 J	<20	<20	<20	<20	<20	<20	<20

^{a/} PCE = tetrachloroethene, TCE = trichloroethene, DCE = dichloroethene, VC = vinyl chloride.

^{b/} µg/L = micrograms per liter.

^{c/} J-flag indicates the concentration is below the quantification limit but above the method detection limit, and the concentration is estimated.

Geotechnical Data

Altus Sites OU-1 and SS-17

TABLE 3
SUMMARY OF GROUNDWATER GEOCHEMICAL DATA
OU1 BIOWALL DEMONSTRATION
ALTUS AFB, OKLAHOMA

Sample Location	Sample Date	Depth to		pH (su) ^{c/}	Conductivity (mS/cm) ^{d/}	Dissolved	Redox	Total Organic	Dissolved	Total	Dissolved	Total	Nitrate-	Ammonia (mg/L)	Ferrous		Chloride (mg/L)	Bromide (mg/L)	Alkalinity (mg/L)	Methane (µg/L) ^{g/}	Ethane (µg/L)	Ethene (µg/L)	Acetylene (µg/L)	
		Water (feet TOC) ^{a/}	Temp (°C) ^{b/}			Oxygen (mg/L) ^{e/}	Potential (mV) ^{f/}	Carbon (mg/L)	Organic Carbon (mg/L)	Carbon (mg/L)	Inorganic Carbon (mg/L)	Dissolved Solids (mg/L)	Nitrite (as N) (mg/L)		Iron (mg/L)	Sulfate (mg/L)								Sulfide (mg/L)
USEPA Monitoring Data																								
EPAUMP1	11-Apr-07	5.18	16.5	6.81	5.50	1.78	-112	2.43	NA ^{h/}	NA	90.9	NA	0.139	NA	<0.10	1,890	<0.01	351	NA	360	169	<1.9	<2.6	<12
Lab Duplicate	6-Sep-07	NA	21.8	6.96	4.60	0.05	-172	1.96	1.88	78.4	76.5	3380	BQL (0.085) ^{i/}	<0.10	0.50	2,040	<0.01	336	1.5	2,900	NA	NA	NA	NA
	6-Sep-07	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.100	<0.10	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
MP1	11-Apr-07	4.55	16.6	6.31	4.89	2.47	-270	7.93	NA	NA	159	NA	0.351	NA	0.45	245	66	270	NA	1,830	786	<1.9	<2.6	<12
	6-Sep-07	4.7	20.3	6.43	3.79	0.05	-349	18.2	13.2	434	421	2280	BQL (0.083)	3.07	0.40	145	0.39	267	0.44	15,600	NA	NA	NA	NA
MP2	6-Sep-07	5.1	19.4	6.48	5.50	0.06	-289	27.7	20.3	500	480	4020	<0.10	4.39	0.20	1,220	0.59	283	0.29	17,400	NA	NA	NA	NA
MP3	6-Sep-07	5.7	20.4	6.44	4.65	0.05	-185	9.07	8.25	264	256	3460	2,870	0.29	2.95	1,480	0.02	267	1.6	98,000	NA	NA	NA	NA
MP4	11-Apr-07	6.45	16.7	6.37	6.21	2.37	-117	7.74	NA	NA	287	NA	BQL (0.090)	NA	2.60	1,840	0.04	294	NA	960	37	<1.9	<2.6	<12
	6-Sep-07	6.2	18.7	6.48	5.12	0.06	-199	6.62	5.04	244	239	4140	0.133	BQL (0.019)	3.80	1,870	<0.01	309	1.4	95,000	NA	NA	NA	NA

^{a/} feet TOC = fett from top of casing.

^{d/} mS/cm = millisiemens per centimeter.

^{g/} µg/L = micrograms per liter.

^{b/} °C = degrees Centigrade.

^{c/} mg/L = milligrams per liter.

^{h/} NA = not analyzed.

^{c/} su = standard pH units.

^{f/} mV = millivolts.

^{i/} BQL indicates the concentration in prentesis is below the quantification limit but above the method detection limit; the concentration is estimated.

EPA Column Study (Altus SS-17)

Analysis result of column B3 influent (supply bag) and effluent (B3E)
Column B3E sampled 5/15/07

Parameters	Column B3E	Supply bag	Unit
Temp	22.3		C
Conductivity	5892		uS
DO	4.11		mg/L
pH	7.35		
ORP	-105.7		mv
S ²⁻	7.55	0	mg/L
Fe ²⁺	0.04	0	mg/L
TOC	5.39	0.85	mg/L
TC	209	49.1	mg/L
TIC	204	48.3	mg/L
Cl ⁻	812	822	mg/L
SO ₄ ²⁻	1670	2440	mg/L
vinyl chloride	1.59	ND	µg/L
1,1-dichloroethene	1.19	ND	µg/L
methylene chloride	ND	ND	µg/L
trans-1,2-dichloroethene	ND	ND	µg/L
1,1-dichloroethane	ND	ND	µg/L
cis-1,2-dichloroethene	13.5	ND	µg/L
chloroform	ND	ND	µg/L
1,1,1-trichloroethane	ND	ND	µg/L
carbon tetrachloride	ND	ND	µg/L
1,2-dichloroethane	ND	8.5	µg/L
trichloroethene	17.2	2585*	µg/L
Ag	ND	ND	mg/L
Al	0.154	0.345	mg/L
As	0.039	0.035	mg/L
B	5.26	3.95	mg/L
Ba	0.161	0.012	mg/L
Be	BQL(0.001)	ND	mg/L
Ca	436	506	mg/L
Cd	ND	ND	mg/L
Co	BQL(0.002)	ND	mg/L
Cr	BQL(0.002)	0.007	mg/L
Cu	ND	BQL(0.010)	mg/L
Fe	ND	0.067	mg/L
K	9.31	8.81	mg/L
Mg	183	189	mg/L
Mn	BQL(0.003)	ND	mg/L
Mo	BQL(0.001)	0.011	mg/L
Na	790	815	mg/L
Ni	ND	0.054	mg/L
Pb	ND	ND	mg/L
Sb	0.015	0.019	mg/L
Se	BQL(0.008)	0.020	mg/L
Sr	7.71	7.93	mg/L
Ti	0.007	0.015	mg/L
Tl	0.039	0.042	mg/L
V	ND	0.007	mg/L
Zn	0.050	0.341	mg/L

Column Study Analytical Results																							
Sample Identification	Sample Label	Sample Date	Time Days	MW				Cl ⁻ mg/L	SO ₄ ²⁻ mg/L	N (nitrate+nitrite) mg/L nd<1.2	TOC mg/L	DC mg/L	DOC mg/L	DIC mg/L	Fe ²⁺ mg/L	S ²⁻ mg/L	Temp °C	Conductivity µs/cm	DO mg/L	pH	ORP mV		
				Methane mg/L	Ethylene mg/L	Ethane mg/L	Acetylene mg/L																
		5/15/2007						822	2440	NO SAMPLE	0.85	49		48									
B3 Effluent	B3E	10/18/2004	1	0.242	ND	ND	ND	872	935	ND	1439.74		1340.00		9.75	0.13	22.1	4543	0.23	6.55	-280		
		11/15/2004	29	4.310	ND	ND	ND	783	582	ND	139.40		112.82		0.80	0.79	22.7	4061	0.30	6.73	-258		
		12/22/2004	66	2.500	ND	ND	ND	723	368	ND	49.80		42.30		0.45	8.50	22.6	3375	0.10	6.64	-313		
		1/24/2005	99	4.880	ND	ND	ND	752	595	ND	33.17		26.72		0.10	15.00	23.2	4099	0.08	6.68	-275		
		2/22/2005	128	6.410	ND	ND	ND	679	588	0.75	169.25		165.81		0.25	7.25	21.9	3248	0.05	6.85	-233		
		3/23/2005	157	3.960	ND	ND	ND	709	835	ND	19.15		14.70		0.15	7.25	23.0	2524	0.05	7.01	-246		
		4/22/2005	187	3.370	ND	ND	ND	652	709	ND	19.00		15.80		0.20	4.10	22.6	3350	0.04	7.08	-275		
		5/23/2005	218	2.990	ND	ND	ND	661	699	ND	12.90		11.20		0.00	4.40	22.9	2856	0.04	7.14	-274		
		6/23/2005	249	6.700	ND	ND	ND	707	773	0.58	17.50		12.50		0.00	6.40	22.7	3120	0.19	7.19	-291		
		9/2/2005	320	6.270	ND	ND	ND	750	612	ND	17.29		14.51		0.00	11.75	22.5	4694	0.09	7.29	-370		
		11/4/2005	383	3.540	ND	ND	ND	780	1110	ND	11.77		10.04		0.00	15.25	22.8	5184					
		1/29/2006	469																				
		3/1/2006	500										10.50							7.07	-276		
		5/18/2006	578										28.70						3.39	6.95	-175		
		6/26/2006	617										9.43		8.05	0.10	0.00	15.9	6922	1.28	7.30	-240	
		7/24/2006	645	1.310	ND	ND	ND						8.57		7.18	0.00	1.37	22.5	5374	1.20	7.27	-275	
		8/21/2006	673	0.795	ND	ND	ND	666	1320	ND	7.25		7.25		6.71	0.05	11.25	22.2	5637	1.30	7.42	-252	
		9/18/2006	701	1.370	ND	ND	ND	680	1510	ND	6.95		6.95		5.98	0.00	11.00	21.1	5716	2.62	7.34	-214	
		10/24/2006	737	1.93	ND	ND	ND									0.00	7.75	21.7	6191	2.41	7.27	-261.50	
		11/20/2006	764					706	1500	ND	6.88		6.88		6.55	0.00	4.50	21.9	6428	3.15	7.05	198	
		12/19/2006	793					709	1450	ND	7.86		7.86		6.05	0.00	9.75	21.5	6532	1.71	7.34	-213	
		2/21/2007	857					721	1690	ND	6.00	215	6.00	215	5.31	210	0.00	16.00	21.9	5854	1.42	6.76	-174
		4/23/2007	918					750	1600	ND													
		5/15/2007	940					812	1670	NO SAMPLE	5.39	209			204								

Dover AFB

TABLE 5
SUMMARY OF GROUNDWATER GEOCHEMICAL DATA
SITE WP-14 BIOWALL DEMONSTRATION
DOVER AFB, DELAWARE

Sample Location	location Description	Sample Date	Temp (°C) ^{a/}	pH (su) ^{b/}	Conductivity (µS/cm) ^{c/}	Dissolved Oxygen (mg/L) ^{d/}	Redox Potential (mV) ^{e/}	Total Organic Carbon (mg/L)	Nitrite+ Nitrate ^{f/} (mg/L)	Nitrate ^{f/} (mg/L)	Nitrite ^{f/} (mg/L)	Manganese (mg/L)	Ferrous Iron (mg/L)	Sulfate (mg/L)	Sulfide (mg/L)	Chloride (mg/L)	Carbon Dioxide (mg/L)	Alkalinity (mg/L)	Total Dissolved Solids (mg/L)	Methane (µg/L) ^{g/}	Ethane (µg/L)	Ethene (µg/L)	Acetylene (µg/L)
Common Background Monitoring Well																							
GSCP9A	25 feet upgradient	1/19/2005	13.3	4.87	96	1.50	+245	4.1	<0.05	<0.05	<0.001	<0.1	0.81	16	0.01	8.8	198	16.4	NA	450	0.920	1.300	NA
Duplicate		1/19/2005	NA ^{h/}	NA	NA	NA	NA	3.9	<0.05	<0.05	0.001	<0.1	0.83	15	0.02	8.8	NA	15.0	NA	480	0.970	1.400	NA
		2/16/2005	19.4	4.22	1342	3.20	+288	<5.0	<0.05	<0.05	0.002	0.3	0.37	22	0.01	3.0	182	12.3	NA	260	0.620	0.830	NA
Duplicate		2/16/2005	NA	NA	NA	NA	NA	<5.0	0.074	0.070	<0.001	0.2	0.37	18	<0.01	<1.0	182	12.3	NA	230	0.590	0.860	NA
		3/30/2005	12.5	5.11	98	2.49	+191	3.9	0.122	0.116	0.006	2.1	0.15	18	0.10	6.6	162	11.1	NA	2	0.079	0.076	NA
Duplicate		3/30/2005	NA	NA	NA	NA	NA	4.0	NA	NA	0.006	2.0	0.16	19	0.11	6.8	162	11.2	NA	NA	NA	NA	NA
		4/21/2005	18.2	4.36	1761	2.45	+371	<5.0	0.140	0.137	0.003	0.8	0.02	19	0.01	8.8	126	10.8	NA	NA	NA	NA	NA
Duplicate		4/21/2005	NA	NA	NA	NA	NA	<5.0	0.220	0.216	0.004	0.6	0.30	20	0.01	8.7	124	10.6	NA	NA	NA	NA	NA
		5/25/2005	11.4	5.07	84	2.06	+87	3.2	0.227	0.223	0.004	1.6	0.04	16	0.01	6.8	160	10.4	NA	2	0.080	0.040	NA
Duplicate		5/25/2005	NA	NA	NA	NA	NA	3.3	NA	NA	0.002	1.4	0.04	16	0.01	7.2	164	10.2	NA	2	0.090	0.110	NA
		6/22/2005	14.4	5.13	87	2.03	+315	10	0.190	0.188	0.002	0.7	0.01	14	<0.01	8.0	70	14.0	NA	NA	NA	NA	NA
Duplicate		6/22/2005	NA	NA	NA	NA	NA	20	0.190	0.188	0.002	NA	<0.01	17	<0.01	7.5	76	13.7	NA	NA	NA	NA	NA
		7/20/2005	17.9	4.70	51	2.39	+381	3.1	0.410	0.408	0.002	0.9	0.03	15	<0.01	6.9	162	11.5	NA	1	0.110	0.040	NA
Duplicate		7/20/2005	NA	NA	NA	NA	NA	3.9	NA	NA	0.003	0.9	0.02	15	<0.01	6.8	156	11.4	NA	1	0.100	0.030	NA
		12/9/2005	13.3	5.53	114	4.85	+212	1.5	0.20	0.190	0.010	0.2	0.10	9.5	<0.01	2.0	35	9.1	NA	2	0.032	0.160	NA
Duplicate		12/9/2005	NA	NA	NA	NA	NA	1.5	NA	NA	0.019	0.1	0.09	9.5	<0.01	2.4	33	8.9	NA	1	0.036	0.150	NA
		6/8/2006	17.1	5.54	52	1.16	+61	NA	0.255	NA	NA	NA	NA	9.7	NA	3.7	NA	NA	NA	15	<1.3	<1.2	NA
North Transect Monitoring Wells																							
TS-MW11	5 feet upgradient	12/12/2004	19.5	5.52	2,077	1.51	+167	<5.0	<0.05	<0.05	0.007	0.5	0.12	12	0.10	6.9	123	25.7	NA	470	0.160	0.630	NA
	east transect	1/18/2005	17.0	5.36	1,778	1.21	+163	1.3	<0.05	<0.05	0.001	1.7	1.8	9.9	0.07	9.2	122	39.8	NA	300	0.078	0.290	NA
		2/10/2005	11.8	5.56	112	0.3	+238	<5.0	<0.05	<0.05	0.002	0.6	0.06	9.0	0.07	7.7	260	33.3	NA	350	0.036	0.190	NA
		3/30/2005	12.4	5.49	119	0.6	+138	4.5	<0.01	<0.01	0.006	1.1	0.18	7.6	0.09	7.2	276	22.1	NA	200	0.044	0.180	NA
		4/18/2005	17.8	4.35	1,830	1.65	+208	8.3	<0.05	<0.05	<0.001	0.7	0.34	10	0.02	9.3	186	35.5	NA	NA	NA	NA	NA
		5/25/2005	11.8	5.69	106	0.53	+173	5.0	0.010 J	0.010 J ^{i/}	<0.001	0.4	0.47	6.8	0.01	7.8	106	31.4	NA	410	0.100	1.400	NA
		6/21/2005	13.0	5.25	98	0.48	+222	36	<0.05	<0.05	0.002	1.6	0.38	5.7	<0.01	8.5	276	26.2	NA	NA	NA	NA	NA
		7/20/2005	18.5	4.94	62	0.54	+246	4.8	0.024	0.024	<0.001	0.1	0.48	3.9	<0.01	7.9	190	34.4	NA	420	0.080	1.500	NA
		12/9/2005	14.2	5.46	111	0.30	+53	6.3	0.020 J	0.008	0.012	0.1	1.3	3.8	<0.01	9.1	146	33.7	NA	740	0.120	1.200	NA
		3/18/2008	12.5	5.27	74	0.28	+60	3.0 J	<0.100	NA	NA	0.4	1.1	6.4	1.0 J	9.4	322	18.7	83	1,200	0.036	0.170	<0.500
	(duplicate)	3/18/2008	NA	NA	NA	NA	NA	3.2 J	<0.100	NA	NA	NA	NA	4.0	1.0 J	9.2	NA	NA	69	1,200	0.025 J	0.040	<0.500
TS-MW01	in upgradient wall	12/12/2004	19.6	6.20	2,010	0.75	-47	59	<0.05	<0.05	<0.001	<0.1	5.9	30	0.04	1.1	384	159	NA	200	0.140	0.760	NA
	north transect	1/18/2005	13.5	6.14	1,554	0.94	-100	100	<0.05	<0.05	<0.001	7.0	20	140	0.07	18	518	697	NA	1,100	0.210	1.800	NA
		2/10/2005	11.9	6.64	1,212	0.01	-130	150	<0.05	<0.05	<0.001	26	35	8.1	0.03	12	744	616	NA	3,600	0.160	1.200	NA
		3/30/2005	13.0	NM	1,187	1.36	-79	110	0.214	0.210	<0.001	18	33	1.4 J	0.03	15	654	616	NA	5,600	0.100	0.600	NA
		4/18/2005	16.3	5.64	1,940	1.30	-135	64	<0.05	<0.05	<0.001	5.4	26	3.8	0.21	13	596	286	NA	NA	NA	NA	NA
		5/25/2005	12.3	6.98	702	0.87	-80	66	0.305	0.310	<0.001	14	23	1.8 J	0.09	11	596	430	NA	13,000	0.070	0.510	NA
		6/20/2005	13.9	6.17	619	1.05	-52	86	<0.05	<0.05	<0.001	36	34	3.5	0.10	11	822	362	NA	NA	NA	NA	NA
		7/19/2005	16.6	5.53	372	0.23	-21	14	0.02	0.02	<0.001	0.7	21	2.8	0.40	9.5	658	208	NA	10,000	<0.03	0.340	NA
		12/8/2005	13.8	6.05	331	0.31	-126	13	0.085	0.081	0.004	0.5	25	7.3	0.50	9.3	920	2174	NA	11,000	0.061	0.510	NA
		3/18/2008	13.6	5.92	448	0.59	-77	16	<0.100	NA	NA	15.5	2.32	3.5	1.3 J	12	272	1050	350	10,000	0.083	0.078	<0.500
TS-MW02	between walls	12/14/2005	19.2	5.29	1,873	1.83	+252	<5.0	<0.05	<0.05	0.002	1.4	0.02	5.1	0.12	7.0	120	20.5	NA	360	0.310	0.510	NA
	north transect	1/18/2005	13.3	5.69	102	2.14	+109	<1.0	<0.05	<0.05	<0.001	0.10	0.01	6.0	0.02	8.5	138	29.2	NA	150	0.200	0.400	NA
		2/10/2005	12.3	5.16	93	<0.01	-142	<5.0	<0.05	<0.05	0.002	0.90	0.07	7.4	0.06	7.9	240	25.3	NA	220	0.180	0.310	NA
		3/30/2005	12.3	5.47	254	2.13	+254	4.7	0.010	0.010	0.001	0.90	0.04	13	0.02	7.6	193	31.1	NA	4	0.013	0.028	NA
		4/18/2005	16.4	4.42	1,954	1.24	+306	6.1	<0.05	<0.05	0.002	0.30	0.01	12	0.01	9.3	298	24.3	NA	NA	NA	NA	NA
		5/25/2005	11.6	5.60	119	0.94	+380	5.0	0.02 J	0.011	0.006	0.90	0.09	9.1	0.05	7.6	208	28.2	NA	200	0.070	0.290	NA
		6/20/2005	14.5	5.38	105	0.71	+258	43	<0.05	<0.05	0.006	1.50	0.12	8.4	<0.01	8.1	210	25.9	NA	NA	NA	NA	NA
		7/20/2005	16.6	4.80	65	0.54	+271	3.7	0.200	0.199	0.001	0.70	0.10	7.9	<0.01	7.4	231	29.9	NA	230	0.035	0.600	NA
		12/9/2005	13.8	5.50	96	0.95	+85	5.0	0.012	0.005	0.007	<0.1	0.48	8.0	<0.01	6.5	289	28.0	NA	730	0.055	0.850	NA
		3/19/2008	14.2	5.58	171	0.39	+96	5.0 J	<0.100	NA	NA	<0.1	1.95	15	1.0 J	9.7	286	84.0	210	2,600	0.029	0.100	<0.100

TABLE 5
SUMMARY OF GROUNDWATER GEOCHEMICAL DATA
SITE WP-14 BIOWALL DEMONSTRATION
DOVER AFB, DELAWARE

Sample Location	location Description	Sample Date	Temp (°C) ^{a/}	pH (su) ^{b/}	Conductivity (µS/cm) ^{c/}	Dissolved Oxygen (mg/L) ^{d/}	Redox Potential (mV) ^{e/}	Total Organic Carbon (mg/L)	Nitrite+Nitrate ^{f/} (mg/L)	Nitrate ^{f/} (mg/L)	Nitrite ^{f/} (mg/L)	Manganese (mg/L)	Ferrous Iron (mg/L)	Sulfate (mg/L)	Sulfide (mg/L)	Chloride (mg/L)	Carbon Dioxide (mg/L)	Alkalinity (mg/L)	Total Dissolved Solids (mg/L)	Methane (µg/L) ^{g/}	Ethane (µg/L)	Ethene (µg/L)	Acetylene (µg/L)
TS-MW03	in down gradient wall north transect	12/12/2004	19.1	6.30	1,916	0.82	-32	97	<0.05	<0.05	0.012	0.3	5.2	1,300	0.07	21	368	NA	NA	190	0.200	1.200	NA
		1/18/2005	13.6	6.33	3,092	0.91	-94	210	<0.05	<0.05	0.11	27	122	300	0.03	27	NA	1,480	NA	2,600	0.210	2.100	NA
		2/15/2005	14.1	6.00	1,876	<0.01	-176	300	<0.05	<0.05	0.049	50	111	15	0.06	22	NA	2,185	NA	7,100	0.280	1.500	NA
		3/30/2005	13.0	6.47	3,905	NA	-116	371	0.423	0.357	0.066	34	181	1.3 J	0.03	28	NA	2,490	NA	8,200	0.110	0.600	NA
		4/22/2005	18.0	6.18	1,827	1.21	-187	340	<0.05	NA	NA	16	142	6.0	0.03	31	NA	1,750	NA	NA	NA	NA	NA
		5/24/2005	14.1	6.43	3,046	1.19	-95	254	0.367	0.370	<0.001	9.0	157	2.7	0.02	22	NA	1,850	NA	7,900	0.100	0.440	NA
		6/20/2005	14.6	6.50	2,707	1.47	-85	230	<0.05	<0.05	<0.001	32	150	5.2	<0.01	15	NA	1,890	NA	NA	NA	NA	NA
		7/20/2005	19.0	5.97	1,640	0.35	-60	140	0.086	0.086	<0.001	43	103	3.5	<0.01	23	NA	1,545	NA	7,200	<0.03	0.300	NA
		12/8/2005	13.1	6.54	1,523	0.42	-136	73	0.14	NA	0.45	3.0	78	5.6	<0.01	17	NA	1,295	NA	9,300	0.100	0.470	NA
TS-MW04	15 feet down gradient north transect	3/19/2008	13.9	6.17	845	0.36	-95	33	<0.100	NA	NA	40	1.9	7.5	1.6 M	12	536	1,100	570	10,000	0.380	0.120	<0.500
		12/12/2004	18.9	5.16	1,913	1.65	+286	<5.0	<0.05	<0.05	0.001	<0.10	0.04	4.5	0.15	7.0	165	25.1	NA	380	0.370	0.440	NA
		1/19/2005	12.4	4.93	73	1.71	+314	<1.0	0.076	0.076	<0.001	0.20	0.03	8.8	0.03	7.5	115	20.9	NA	78	0.100	0.130	NA
		2/10/2005	26.7	4.61	1,472	7.73	+321	<5.0	0.200	0.195	0.005	0.60	0.09	9.3	0.08	6.6	176	16.8	NA	71	0.058	0.220	NA
		3/29/2005	11.6	5.42	83	0.99	+306	1.6	0.099	0.097	0.002	0.40	0.15	9.3	0.21	7.2	169	17.7	NA	7	0.014	0.031	NA
		4/19/2005	14.9	4.55	1,464	0.14	+329	<5.0	0.080	0.076	0.004	0.50	0.01	11	0.02	9.8	92	14.6	NA	NA	NA	NA	NA
		5/24/2005	12.7	4.80	86	0.56	+343	1.1	0.090	0.083	0.007	0.70	0.04	7.7	0.03	8.2	111	14.2	NA	69	0.040	0.290	NA
		6/20/2005	14.2	5.27	80	0.59	+253	14	0.070	0.065	0.005	1.80	0.07	8.7	<0.01	9.3	137	13.2	NA	NA	NA	NA	NA
		7/19/2005	15.6	4.45	76	0.33	+442	0.30	0.028 J	0.024 J	0.004	1.10	<0.10	8.1	<0.01	9.7	75	14.8	NA	40	0.02 J	0.160	NA
TS-MW05	30 feet down gradient north transect	12/8/2005	14.9	5.76	119	0.85	+114	3.9	0.039 J	0.038	0.001	0.20	0.84	14	<0.01	11	139	29.3	NA	170	0.045	0.260	NA
		3/19/2008	13.3	5.59	133	0.24	+118	2.5 J	<0.100	NA	NA	<0.1	<0.01	9.2	1.0 J	9.8	296	70	120	1,300	0.022	0.330	<0.500
		12/15/2004	17.1	5.52	1,730	1.15	+188	<5.0	<0.05	<0.05	0.014	<0.1	0.10	5.1	0.01	6.3	153	26.7	NA	280	0.370	0.620	NA
		1/19/2005	12.9	5.16	108	2.65	+239	<1.0	<0.05	<0.05	<0.001	<0.1	0.07	6.2	<0.01	8.3	166	28.3	NA	350	0.230	0.350	NA
		2/10/2005	18.8	4.53	1,371	0.04	+242	<5.0	<0.05	<0.05	0.003	0.5	0.11	6.0	0.02	7.6	236	25.0	NA	440	0.110	0.390	NA
		3/29/2005	12.0	5.53	90	1.17	+269	3.1	0.014	0.013	0.001	0.4	0.02	3.1	0.02	7.1	254	27.4	NA	3.3	0.015	0.021	NA
		4/19/2005	14.8	4.19	1,495	0.49	+346	<5.0	<0.05	<0.05	0.003	1.1	0.05	5.8	0.02	8.8	198	25.7	NA	NA	NA	NA	NA
		5/24/2005	13.1	4.87	121	0.44	+268	3.6	0.024J	0.024J	<0.001	0.9	0.90	18	0.03	7.5	71	24.0	NA	320	0.050	0.810	NA
		6/20/2005	13.7	5.25	98	0.89	+206	26	<0.05	<0.05	0.001	1.1	0.14	11	<0.01	7.8	222	23.1	NA	NA	NA	NA	NA
South Transect Monitoring Wells (Amended with Sulfate)	10 feet upgradient south transect	7/19/2005	18.1	4.72	112	0.37	+334	3.9	0.028 J	0.023 J	0.005	0.6	0.07	12	<0.01	8.3	228	26.5	NA	1,800	0.02 J	0.590	NA
		12/7/2005	14.6	5.78	247	0.53	-30	8.6	0.024 J	0.023	0.001	0.1	2.9	5.5	<0.01	9.7	258	48.4	NA	580	0.170	1.000	NA
		12/15/2004	20.6	5.34	1,537	0.74	+188	<5.0	<0.05	<0.05	0.016	0.3	0.17	13	<0.01	4.2	188	17.2	NA	120	0.260	0.410	NA
		12/15/2004	NA	NA	NA	NA	NA	<5.0	<0.05	<0.05	0.019	0.4	0.12	12	<0.01	4.2	175	17.8	NA	85	0.230	0.310	NA
		1/19/2005	12.7	5.14	100	0.85	-7	<1.0	<0.05	<0.05	0.002	0.7	0.02	14	<0.01	6.1	105	23.9	NA	34	0.016	0.056	NA
		2/15/2005	18.5	4.82	1,375	4.14	+250	<5.0	<0.05	<0.05	<0.001	0.5	0.06	14	0.07	6.2	132	25.5	NA	12	<0.005	0.053	NA
		3/29/2005	12.3	5.57	111	4.07	+282	1.9	<0.04	<0.04	0.009	1.5	<0.01	18	0.02	4.3	160	26.0	NA	1.8	0.010	0.026	NA
		4/22/2005	16.5	4.81	2,188	7.32	+309	<5.0	0.060	0.053	0.007	1.2	0.03	28	0.05	<1.0	77	22.7	NA	NA	NA	NA	NA
		5/24/2005	17.1	5.12	126	5.61	+375	1.5	0.092	0.087	0.005	2.5	0.04	24	0.03	4.5	105	22.3	NA	3	0.01 J	0.050	NA
TS-MW06	in upgradient wall south transect	6/20/2005	13.7	5.37	118	5.37	+315	13	<0.05	<0.05	0.002	0.8	0.05	25	<0.01	5.8	162	21.3	NA	NA	NA	NA	NA
		7/18/2005	17.6	4.62	117	4.73	+422	1.8	0.150	0.142	0.008	0.6	0.06	31	<0.10	4.6	160	21.0	NA	5.5	<0.03	0.02 J	NA
		12/6/2005	14.2	6.10	220	0.66	+267	2.4	0.110	0.105	0.005	0.4	0.07	76	<0.01	5.1	227	28.3	NA	4.2	0.008 J	0.130	NA
		3/18/2008	13.1	5.21	113	0.39	+239	1.5 J	0.320	NA	NA	0.4	<0.01	34	0.60 J	6.5	267	18.0	110	86	0.006 J	0.022 J	<0.500
		12/15/2004	17.8	6.27	1,409	3.95	-8	34	<0.05	<0.05	0.01	0.9	7.7	1,100	0.03	8.0	380	218	NA	78	0.120	0.740	NA
		1/20/2005	13.2	7.15	669	2.94	-41	9.5	<0.05	<0.05	<0.001	38	31	440	0.02	8.2	526	275	NA	320	0.050	0.490	NA
		2/15/2005	20.0	5.59	1,289	5.15	-57	10	0.051	0.050	<0.001	43	24	410	0.07	6.7	614	409	NA	400	0.023	0.270	NA
		3/29/2005	11.2	6.04	455	4.09	+82.6	3.1	0.063	0.059	0.004	2.9	2.4	149	0.05	4.9	288	126	NA	3	0.018	0.031	NA
		4/22/2005	14.3	5.36	1,519	2.57	-32	7.6	<0.05	<0.05	0.002	4.0	5.5	230	0.01	7.5	358	222	NA	NA	NA	NA	NA
		5/24/2005	12.8	6.09	758	3.31	-84	3.5	0.107	0.104	0.003	3.1	2.8	182	0.01	5.1	196	228	NA	180	0.02 J	0.090	NA
		6/21/2005	15.2	6.19	818	3.08	-23	29	<0.5	<0.05	0.002	2.9	4.0	190	0.5	6.2	280	273	NA	NA	NA	NA	NA
		7/19/2005	18.0	5.82	586	2.57	+20	4.1	0.13	0.13	<0.001	0.1	0.03	150	0.1	5.4	244	130	NA	150	0.006	0.064	NA
		12/7/2005	14.3	6.00	529	NA	-57	24	0.078	0.067	0.011	9.3	13	320	<0.01	6.6	1024	580	NA	660	0.074	0.720	NA
		3/18/2008	12.5	6.06	768	0.57	-215	2.8 J	0.57	NA	NA	2.9	2.5	530	3.2	6.5	167	356	680	2,200	0.006 J	0.120	<0.500

TABLE 5
SUMMARY OF GROUNDWATER GEOCHEMICAL DATA
SITE WP-14 BIOWALL DEMONSTRATION
DOVER AFB, DELAWARE

Sample Location	location Description	Sample Date	Temp (°C) ^{a/}	pH (su) ^{b/}	Conductivity (µS/cm) ^{c/}	Dissolved Oxygen (mg/L) ^{d/}	Redox Potential (mV) ^{e/}	Total Organic Carbon (mg/L)	Nitrite+Nitrate ^{f/} (mg/L)	Nitrate ^{f/} (mg/L)	Nitrite ^{f/} (mg/L)	Manganese (mg/L)	Ferrous Iron (mg/L)	Sulfate (mg/L)	Sulfide (mg/L)	Chloride (mg/L)	Carbon Dioxide (mg/L)	Alkalinity (mg/L)	Total Dissolved Solids (mg/L)	Methane (µg/L) ^{g/}	Ethane (µg/L)	Ethene (µg/L)	Acetylene (µg/L)
TS-MW07	between walls south transect	12/15/2004	19.4	5.40	1,341	1.44	+232	<5.0	<0.05	<0.05	0.001	<0.1	0.04	14	<0.01	5.0	201	21.2	NA	230	0.150	0.410	NA
		1/20/2005	12.1	5.52	110	1.55	+192	<1.0	<0.05	<0.05	<0.001	0.1	<0.01	15	0.04	6.7	116	29.0	NA	93	0.012	0.300	NA
		2/15/2005	20.3	4.85	1,282	4.90	+248	<5.0	<0.05	<0.05	0.004	0.3	0.03	14	0.02	6.1	132	30.0	NA	74	0.046	0.370	NA
		3/29/2005	11.8	5.47	64	2.08	+260	0.9 J	<0.01	<0.01	0.001	0.5	0.05	12	0.05	4.4	130	30.0	NA	2	0.015	0.035	NA
		4/22/2005	16.0	4.50	1,435	0.55	+304	<5.0	<0.05	<0.05	0.002	0.9	0.03	17	0.01	7.0	94	18.0	NA	NA	NA	NA	NA
		5/23/2005	13.8	4.90	84	0.61	+324	1.1	0.016J	0.013J	0.003	0.6	<0.01	12	0.01	4.4	120	22.0	NA	46	0.01 J	0.090	NA
		6/21/2005	14.8	5.37	83	0.58	+273	29	<0.05	<0.05	<0.001	1.2	0.02	12	<0.01	6.1	208	8.0	NA	NA	NA	NA	NA
		7/19/2005	16.5	5.08	116	0.42	+301	3.1	0.019 J	0.016 J	0.003	0.7	0.08	42	<0.01	5.2	168	26.0	NA	100	0.013	0.250	NA
		12/7/2005	14.6	4.65	358	NA	+261	17	0.011 J	0.003	0.008	1.0	0.34	430	<0.01	11	776	152	NA	500	0.062	0.330	NA
		3/20/2008	13.1	5.89	1,715	0.97	+63	5.3	<0.100	NA	NA	>22	1.32	970	1.3 J	7.9	>500	390	1,900	3,300	0.022 J	0.790	<0.500
TS-MW08	in down gradient wall south transect	12/16/2004	19.1	6.42	1,628	0.85	-47	75	<0.05	<0.05	0.008	<0.1	9.4	1,100	0.02	19	239	264	NA	100	0.180	1.300	NA
		1/20/2005	12.4	6.36	4,007	1.87	-105	180	<0.05	<0.05	0.070	NA	63	1,400	0.12	30	448	1,700	NA	1,300	0.440	4.100	NA
		2/15/2005	19.9	5.98	1,320	1.49	-153	84	<0.05	<0.05	<0.001	4.0	41	450	0.02	14	1,080	1,115	NA	1,100	0.660	2.000	NA
		3/29/2005	11.8	6.18	3,258	7.64	-75	70	0.121	0.121	<0.001	31	31	682	0.04	18	1,574	1,490	NA	900	0.410	1.100	NA
		4/22/2005	17.1	6.01	1,915	0.48	-162	80	<0.05	<0.05	<0.001	22	29	560	0.90	9.0	1,314	1,070	NA	NA	NA	NA	NA
		5/23/2005	15.4	6.47	3,009	0.73	-66	48	0.213	0.213	<0.001	29	26	530	0.02	15	1,618	1,250	NA	1,800	0.270	0.840	NA
		6/21/2005	16.4	6.40	3,012	1.44	-79	210	<0.05	<0.05	<0.001	4.0	26	660	<0.01	15	1,676	1,425	NA	NA	NA	NA	NA
		7/18/2005	17.4	5.91	2,231	0.3	-86	36	0.067	0.067	<0.001	3.0	21	490	<0.01	13	1,096	1,315	NA	1,600	0.160	0.780	NA
		12/8/2005	11.7	6.50	2,353	0.76	-159	55	0.018 J	NA	0.037	13	10	570	0.1	34	1,854	1,270	NA	1,600	0.190	1.400	NA
		3/20/2008	13.5	6.12	3,930	NA	-375	63	0.230	NA	NA	40	0.27	1,000	51.0	<1.0	>500	640	4,500	2,800	0.075	2.000	<0.500
TS-MW09	15 feet down gradient south transect	12/16/2004	19.6	NA	1,510	2.43	+249	<5.0	0.800	0.794	0.006	0.4	0.16	18	0.04	5.0	170	18.7	NA	180	0.400	0.670	NA
		1/20/2005	12.1	4.97	82	1.13	+292	<1.0	<0.05	<0.05	<0.001	0.4	<0.01	14	0.01	6.8	112	16.7	NA	120	0.052	0.081	NA
		2/16/2005	19.6	4.91	1,987	0.06	+268	<5.0	<0.05	<0.05	<0.001	0.7	0.10	13	0.01	6.1	230	18.2	NA	61	<0.005	0.100	NA
		3/28/2005	11.5	5.32	95	7.05	+317	0.6 J	<0.01	<0.01	0.008	<0.1	0.05	21	0.02	4.3	60	12.3	NA	2	0.029	0.031	NA
		4/22/2005	16.9	4.50	1,827	0.59	+336	<5.0	<0.05	<0.05	0.002	0.8	0.04	18	0.03	6.7	120	20.0	NA	NA	NA	NA	NA
		5/23/2005	13.6	5.20	101	3.05	+374	1.3	0.021 J	0.017 J	0.004	1.1	0.05	24	0.01	4.5	82	16.0	NA	8	0.02 J	0.070	NA
		6/21/2005	14.0	5.22	169	1.49	+285	13	0.080	0.080	<0.001	2.9	0.09	55	<0.01	6.2	201	24.0	NA	NA	NA	NA	NA
		7/18/2005	17.2	4.68	162	0.60	+304	1.8	0.060	0.058	0.002	1.4	0.07	58	<0.01	4.7	184	14.0	NA	25	0.02 J	0.140	NA
		12/6/2005	15.2	5.84	302	0.34	+280	4.8	0.057	0.053	0.004	0.7	0.13	150	<0.01	9.7	308	46.0	NA	150	0.032	0.120	NA
		3/17/2008	13.6	5.50	848	0.41	+121	5.9	0.650	NA	NA	2.6	1.82	430	0.6 J	7.1	726	2.8	690	460	0.014 J	0.040	<0.500
TS-MW10	25 feet down gradient south transect	12/16/2004	16.1	NA	1,505	5.10	+408	<5.0	0.560	0.555	0.005	0.1	0.05	43	0.03	5.2	73	14.7	NA	3	0.120	0.240	NA
		1/19/2005	11.3	5.00	96	3.30	+361	<1.0	0.170	0.170	<0.001	<0.1	<0.01	25	<0.01	6.7	121	8.5	NA	11	0.230	0.300	NA
		2/16/2005	20.1	4.44	1,287	6.44	+343	<5.0	0.140	0.136	0.004	0.6	0.03	18	<0.01	<1.0	141	12.6	NA	18	0.050	0.096	NA
		3/28/2005	10.9	4.67	91	5.73	+374	2.1	0.138	0.137	0.001	0.2	<0.01	18	0.01	5.1	126	13.7	NA	1	0.014	0.022	NA
		4/22/2005	14.5	4.04	1,510	0.67	+368	<5.0	0.080	0.077	0.003	1.4	0.03	15	<0.01	7.5	100	14.6	NA	NA	NA	NA	NA
		5/23/2005	12.3	5.12	109	0.73	+315	2.7	0.109	0.106	0.003	0.7	0.11	15	<0.01	5.6	149	18.0	NA	320	0.500	1.400	NA
		6/21/2005	13.4	5.16	92	1.78	+261	16	0.190	0.187	0.003	1.8	0.21	15	<0.01	7.0	144	15.0	NA	NA	NA	NA	NA
		7/18/2005	15.2	4.66	79	0.51	+281	2.7	0.100	0.097	0.003	0.5	0.15	14	<0.01	5.9	68	16.0	NA	270	0.240	0.690	NA
		12/6/2005	15.8	5.08	201	0.45	+404	3.8	0.450	0.444	0.006	0.2	0.03	74	<0.01	6.1	236	17.0	NA	26	0.013 J	0.120	NA

^{a/} °C = degrees Centigrade.

^{b/} su = standard pH units.

^{c/} µS/cm = microsiemens per centimeter.

^{d/} mg/L = milligrams per liter.

^{e/} mV = millivolts.

^{f/} Nitrate+Nitrite analyzed by USEPA Method E353.3.
Nitrite measured separately using Hach Method 8507.

^{g/} µg/L = micrograms per liter.

^{h/} NA = not analyzed.

^{i/} J-flag indicates the concentration is estimated.

TABLE 6
CATIONS/ANIONS IN GROUNDWATER
SITE WP-14 BIOWALL DEMONSTRATION
DOVER AFB, DELAWARE

Sample Location	location Description	Sample Date	Chloride (mg/L) ^{a/}	Flouride (mg/L)	Phosphate (mg/L)	Sulfate (mg/L)	Sulfide (mg/L)	Nitrite+Nitrate as Nitrogen (mg/L)	Calcium (mg/L)	Iron (mg/L)	Magnesium (mg/L)	Manganese (mg/L)	Potassium (mg/L)	Sodium (mg/L)
North Transect Monitoring Wells														
TS-MW11	5 feet upgradient	3/18/2008	9.4	0.48 J ^{b/}	0.76 JM ^{c/}	6.4	1.0 J	<0.100	3.4	1.00 M	2.10	0.031	0.780	11.0
Duplicate		3/18/2008	9.2	0.46 J	<1.00 M	4.0	1.0 J	<0.100	3.3	0.97 M	2.00	0.030	0.770	11.0
TS-MW01	In upgradient biowall	3/18/2008	12	0.48 J	<1.00 M	3.5	1.3 J	<0.100	49	45.0 M	22.0	0.590	9.20	14.0
TS-MW02	Between biowalls	3/19/2008	9.7	0.44 J	<1.00 M	15	1.0 J	<0.100	14	1.50 M	8.10	0.098	2.40	15.0
TS-MW03	In downgradient biowall	3/19/2008	12	0.47 J	<1.00 M	7.5	1.6 J	<0.100	120	45.0 M	30.0	0.590	19.0	14.0
TS-MW04	15 feet downgradient	3/19/2008	9.8	0.44 J	<1.00 M	9.2	1.0 J	<0.100	10	0.34 M	6.40	0.140	1.00	12.0
South Transect Monitoring Wells														
TS-MW12	10 feet upgradient	3/18/2008	6.5	0.48 J	0.87 JM	34	0.60 J	0.320	7.4	<0.05	4.900	0.120	1.20	8.0
TS-MW06	In upgradient biowall	3/18/2008	6.50	0.50 J	0.22 JM	530	3.2	0.570	180	2.1 M	27.000	0.300	1.80	9.3
TS-MW07	Between biowalls	3/20/2008	7.90	0.48 J	<1.00	970	1.3 J	<0.100	470	1.0	37.000	2.50	1.80	12.0
TS-MW08	In downgradient biowall	3/28/2008	<1.00	0.49 J	3.00	1,000	51.0	0.230	1,200	1.2	83.000	1.8	43.0	16.0
TS-MW09	15 feet downgradient	3/17/2008	7.1	0.56	<1.000	430	0.6 J	0.650	93	1.7 M	53.000	1.20	1.60	13.0

^{a/} mg/L = milligrams per liter.

^{b/} J-flag indicates the concentration is estimated.

^{c/} M-flag indicates recovery/RPD poor for MS/MSD.

Seneca Depot

TABLE 4
FULL-SCALE GROUNDWATER GEOCHEMICAL DATA
ASH LANDFILL BIOWALL, SENECA ARMY DEPOT ACTIVITY, NEW YORK

Well ID	Location Description	Sample Date	Temperature (°C) ^{a/}	pH (su) ^{a/}	Specific Conductance (mS/cm) ^{a/}	Dissolved Oxygen (mg/L) ^{a/}	ORP (mV) ^{a/}	Total Organic Carbon (mg/L)	Alkalinity (mg/L)	Total Dissolved Solids (mg/L)	Nitrate+Nitrite as Nitrogen (mg/L)	Manganese (mg/L)	Ferrous Iron (mg/L)	Sulfate (mg/L)	Methane (µg/L) ^{a/}	Ethane (µg/L)	Ethene (µg/L)	Acetylene (µg/L)
MWT-25	Upgradient of Biowall A	15-Nov-07	NA	6.90	1.20	0.21	65	NA ^{b/}	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
		10-Jan-08	7.12	7.15	1.10	0.27	2.5	NA	NA	730	NA	NA	NA	NA	NA	NA	NA	NA
TEMP-1	In Biowall A	10-Jan-08	5.63	6.35	1.03	0.3	-96.9	13	390	690	<0.05 M ^{c/}	8.5 M	11	180 M	23,000	2.4	11	<0.500
MWT-26	Upgradient of Biowalls B1/B2	15-Nov-07	NA	7.08	1.90	0.89	-40	6.1	NA	NA	NA	0.0	1.09	1060	44	0.16	0.4	NA
		10-Jan-08	7.51	7.46	1.77	2.96	37.3	NA	NA	1400	NA	NA	NA	NA	NA	NA	NA	NA
MWT-27	In Biowall B1	15-Nov-07	NA	6.43	5.76	0.06	-166	167	NA	NA	NA	22	2.19	31.7	13,000	ND	0.014 J ^{d/}	NA
		9-Jan-08	7.88	6.46	2.60	0.33	-111	NA	NA	1900	NA	NA	NA	NA	NA	NA	NA	NA
MWT-28	In Biowall B2	15-Nov-07	NA	6.48	1.72	0.08	-151	92	NA	NA	NA	22	2.15	ND	11,000	0.014 J	ND	NA
		9-Jan-08	8.22	6.35	1.15	0.49	-139.3	NA	NA	820	NA	NA	NA	NA	NA	NA	NA	NA
MWT-29	Downgradient of Biowall B2	14-Nov-07	NA	7.04	1.88	0.21	-101	20.9	NA	NA	NA	8.6	3.3	289	2,600	19	200	NA
		9-Jan-08	7.61	6.70	1.05	2.11	87.9	NA	NA	750	NA	NA	NA	NA	NA	NA	NA	NA
MWT-22	Downgradient of Biowall B2	14-Nov-07	NA	6.53	1.81	0.18	-132	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
		10-Jan-07	8.57	6.68	1.90	0.26	-43.7	NA	NA	1300	NA	NA	NA	NA	NA	NA	NA	NA
PT-22	Between Biowalls B and C	14-Nov-07	NA	6.73	1.26	0.17	-166	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
		10-Jan-08	8.86	7.44	1.07	0.35	-50.1	NA	NA	670	NA	NA	NA	NA	NA	NA	NA	NA

^{a/} °C = degrees Celsius; su = standard pH units; mS/cm = millisiemens per centimeter; mg/L = milligrams per liter; mV = millivolts; µg/L = micrograms per liter.

^{b/} NA = Not analyzed or not available.

^{c/} M-flag indicates Recovery/RPD poor for MS/MSD.

^{d/} J-flag indicates the concentration is estimated.

NOTE: Analysis of TOC, sulfate, methane, ethane, and ethene were completed for the biowall program monitoring wells only.

TABLE 5
CATIONS/ANIONS IN GROUNDWATER
ASH LANDFILL BIOWALL, SENECA ARMY DEPOT ACTIVITY, NEW YORK

Sample Location	location Description	Sample Date	Total Dissolved		Chloride (mg/L)	Flouride (mg/L)	Phosphate (mg/L)	Sulfate (mg/L)	Sulfide (mg/L)	Nitrate (mg/L)	Nitrite (mg/L)	Calcium (mg/L)	Iron (mg/L)	Magnesium (mg/L)	Manganese (mg/L)	Potassium (mg/L)	Sodium (mg/L)
			Solids (mg/L) ^{a/}														
MWT-25	Upgradient of Biowall A	10-Jan-08	730		33.0	0.60	<1.00 M ^{b/}	190.0	1.3 J ^{c/}	1.20	<0.50	160	0.057 M	33.0	0.36 M	13.0	48.0
TEMP-1	In Biowall A	10-Jan-08	690		29.0	0.56	<1.00 M	180 M	1.9 J	<1.00	0.93	170	13.0 M	18.0	8.5 M	4.30	24.0
MWT-26	Upgradient of Biowalls B1/B2	10-Jan-08	1,400		55.0	0.90	<1.00 M	1,000	1.0 J	1.40	<0.50	230	0.042 JM	49.0	0.010 JM	26.0	120
MWT-36	Duplicate of MWT-26	10-Jan-08	1,400		59.0	0.91	<1.00 M	1,000	1.3 J	1.20	<0.50	220	0.043 JM	50.0	0.010 JM	26.0	120
MWT-27	In Biowall B1	9-Jan-08	1,900		40.0	1.10	<1.00	10.0	0.60 J	0.98	1.1	430	66.0 M	80.0	7.20 M	94.0	50.0
MWT-28	In Biowall B2	9-Jan-08	820		9.2	0.62	<1.00	3.10	1.6 J	1.00	0.41 J	230	27.0 M	32.0	3.7 M	34.0	16.0
MWT-29	Downgradient of Biowall B2	9-Jan-08	750		18.0	0.74	<1.00	220	1.0 J	1.30	<0.50	160	0.100 M	29.0	0.90 M	13.0	44.0
MWT-22	Downgradient of Biowall B2	10-Jan-08	1,300		47.0	<0.50	<1.00 M	100 M	1.6 J	1.00	1.5	310	3.50 M	52.0	5.7 M	8.30	110
PT-22	Between Biowalls B and C	10-Jan-08	670		130.0	0.80	<1.00 M	170 M	1.6 J	0.99	<0.50	130	0.300 M	36.0	0.097 M	9.20	29.0

^{a/} mg/L = milligrams per liter.

^{b/} M-flag indicates Recovery/RPD poor for MS/MSD.

^{c/} J-flag indicates the concentration is estimated.

Dugway PG

TABLE 4
GROUNDWATER GEOCHEMICAL DATA
SWMU-97 PILOT TEST, DUGWAY PROVING GROUND, UTAH

Sample Location	Sample Date	Sample Location	Temp (°C)	pH (su) ^{a/}	Conductivity (mS/cm)	Dissolved Oxygen (mg/L) ^{b/}	Redox Potential (mV) ^{c/}	Dissolved Organic Carbon (mg/L)	Total Dissolved Solids (mg/L)	Nitrate (as N) (mg/L)	Nitrite (as N) (mg/L)	Manganese (mg/L)	Ferrous Iron (mg/L)	Sulfate (mg/L)	Sulfate (mg/L)	Sulfide (mg/L)	Chloride (mg/L)	Chloride (mg/L)	Bromide (mg/L)	Carbon Dioxide (mg/L)	Alkalinity (mg/L)	Methane (µg/L) ^{d/}	Ethane (µg/L)	Ethene (µg/L)
Field Measurement/Fixed-Base Laboratory			Field	Field	Field	Field	Field	Lab - TA	Lab - MS	Lab - TA	Lab - TA	Field	Field	Lab - MS	Lab - TA	Field	Lab - MS	Lab - TA	Lab - TA	Field	Field	Lab - MS	Lab - MS	Lab - MS
TW22	24-Apr-08	Downgradient	13.8	6.20	60.28	0.24	-145	9.3 J,B	59,000	<5.0	<5.0	2.7	6.90	11,000	11,600	0.656	26,000	27,100	<50	549	611	6.30	0.66	1.50
Duplicate	24-Apr-08		NA	NA	NA	NA	NA	8.3 J,B	59,000	<5.0	<5.0	2.8	6.25	12,000	11,700	0.445	26,000	27,400	<50	530	636	8.20	0.66	1.50
TW23	24-Apr-08	Downgradient	13.5	5.69	64.54	1.03	-150	100 B	63,000	<5.0	<5.0	2.3	5.20	11,000	11,200	0.300	28,000	29,600	62	699	1,286	36	0.13	1.30
TW24	22-Apr-08	Downgradient	14.9	5.38	71.53	2.40	238	9.5 J,B	60,000	<5.0	<5.0	0.5	0.15	12,000	11,600	0.003	27,000	29,800	<50	163	249	8.30	0.14	0.44
TW25	22-Apr-08	Upgradient	14.78	6.23	64.28	0.28	64.4	8.6 J,B	57,000	<5.0	<5.0	0.7	0.17	12,000	12,400	0.011	26,000	24,700	<50	178	309	5.10	0.01 J	1.50
TW26	22-Apr-08	Crossgradient	13.8	6.96	67.21	0.17	-115	8.9 J,B	NA	<5.0	<5.0	0.4	0.82	12,000	11,900	0.002	26,000	26,800	<50	159	247	0.26	0.022J	0.62
TW27	22-Apr-08	Crossgradient	14.3	5.49	65.86	0.42	-119	198 B	NA	<5.0	<5.0	2.6	6.55	11,000	10,900	0.065	25,000	25,600	117	515	1,585	240	2.40	1.20
TW28	22-Apr-08	Within Injection Zone	13.9	6.30	65.72	0.85	-203	121 B	54,000	<5.0	<5.0	3.7	5.20	10,000	10,400	1.045	24,000	24,700	95	948	2,341	210	1.30	1.40
TW29	22-Apr-08	Downgradient	13.7	5.44	66.80	0.87	-142	228 B	56,000	<5.0	<5.0	15.1	5.45	11,000	10,800	0.083	22,000	25,900	108	504	1,896	120	1.10	1.20
IW-02	24-Apr-08	Injection Well	12.4	5.42	57.52	NR ^{f/}	-171	3,390 B	59,000	<5.0	<5.0	7.0	4.85	7,900	8,040	1.280	23,000	24,800	162	624	1,878	6.80	0.33	0.47
IW-03	24-Apr-08	Injection Well	13.2	5.17	55.13	NR ^{f/}	-124	4,420 B	62,000	<5.0	<5.0	10.7	4.40	9,000	9,270	0.335	23,000	24,500	193	634	2,117	3.70	0.36	0.56

^{a/} su = standard pH units.

^{b/} mg/L = milligrams per liter.

^{c/} mV = millivolts.

^{d/} µg/L = micrograms per liter.

^{e/} NA = not analyzed or not available.

^{f/} NR = data not reported, dissolved oxygen membrane fouled by oil in well.

TABLE 5
CATIONS/ANIONS IN GROUNDWATER
SWMU-97 PILOT TEST, DUGWAY PROVING GROUND, UTAH

Sample Location	Location Description	Sample Date	Chloride (mg/L) ^{a/}	Chloride (mg/L)	Flouride (mg/L)	Flouride (mg/L)	Bromide (mg/L)	Nitrate (as N) (mg/L)	Nitrite (as N) (mg/L)	Phosphate (mg/L)	Phosphate (mg/L)	Sulfate (mg/L)	Sulfate (mg/L)	Sulfide (lab) (mg/L)	Sulfide (field) (mg/L)	Nitrite+Nitrate as Nitrogen (mg/L)	Calcium (mg/L)	Iron (mg/L)	Magnesium (mg/L)	Manganese (mg/L)	Potassium (mg/L)	Sodium (mg/L)
Laboratory			MS	TA	MS	TA	TA	TA	TA	MS	TA	MS	TA	MS	Field	MS	MS	MS	MS	MS	MS	MS
TW-22	Downgradient	4/24/2008	26,000	27,100	<50	<50	<50	<5.0	<5.0	<100	<20	11,000	11,600	<2.0	0.656	NA	850	6.1 M ^{b/}	2,000	1.5	550	15,000
(duplicate)		4/24/2008	26,000	27,400	<50	<50	<50	<5.0	<5.0	<100	<20	12,000	11,700	<2.0	0.445	NA	830	5.9 M	1,900	1.4	530	14,000
TW-23	Downgradient	4/24/2008	28,000	29,600	<50	<50	62	<5.0	<5.0	<100	<20	11,000	11,200	<2.0	0.300	NA	860	11	2,300	1.6	690	16,000
TW-24	Downgradient	4/22/2008	27,000	29,800	<25	<50	<50	<5.0	<5.0	<50	<20	12,000	11,600	<2.0	0.003	NA	770	0.035 J ^{c/}	2,000	0.034	660	18,000
TW-25	Upgradient	4/22/2008	26,000	24,700	<25	<50	<50	<5.0	<5.0	<50	<20	12,000	12,400	<2.0	0.011	NA	760	0.088	2,200	0.092	740	17,000
TW-26	Crossgradient	4/22/2008	26,000	26,800	<25	<50	<50	<5.0	<5.0	<50	<20	12,000	11,900	0.6 J	0.002	NA	760	0.67	2,000	0.34	650	17,000
TW-27	Crossgradient	4/22/2008	25,000	25,600	<25	<50	117	<5.0	<5.0	<50	<20	11,000	10,900	1.9 J	0.065	NA	800	8.6	2,400	0.87	520	18,000
TW-28	Within Injection Zone	4/22/2008	24,000	24,700	<25	<50	95	<5.0	<5.0	<50	<20	10,000	10,400	4.5	1.045	NA	740	4.1	1,900	1.3	530	16,000
TW-29	Downgradient	4/22/2008	22,000	25,900	<25	<50	108	<5.0	<5.0	<50	<20	11,000	10,800	1.9 J	0.083	NA	760	18	2,200	1.2	500	16,000
IW-02	Injection Well	4/24/2008	23,000	24,800	<50	<50	162	<5.0	<5.0	280	65	7,900	8,040	5.2	1.280	NA	890	38 M	2,100	16	580	14,000
IW-03	Injection Well	4/24/2008	23,000	24,500	<50	<50	193	<5.0	<5.0	560	113	9,000	9,270	2.1	0.335	NA	1,200	47 M	2,200	8.600	690	13,000

NOTE: Analyses were performed by TA = Test America or MS = Microseeps, Inc.

^{a/} mg/L = milligrams per liter.

^{b/} M-flag indicates Recovery/RPD poor for MS/MSD.

^{c/} J-flag indicates the concentration is above the method detection limit but below the laboratory reporting limit, the concentration is estimated.

TABLE 6
TOTAL METALS IN GROUNDWATER
SWMU-97 PILOT TEST, DUGWAY PROVING GROUND, UTAH

Sample Location	Location Description	Sample Date	Aluminum (μ/L) ^{a/}	Antimony (μ/L)	Arsenic (μ/L)	Barium (μ/L)	Beryllium (μ/L)	Cadmium (μ/L)	Calcium (μ/L)	Chromium (μ/L)	Cobalt (μ/L)	Copper (μ/L)	Iron (μ/L)	Lead (μ/L)	Magnesium (μ/L)	Manganese (μ/L)	Molybdenum (μ/L)	Nickel (μ/L)	Potassium (μ/L)	Selenium (μ/L)	Silver (μ/L)	Sodium (μ/L)	Thallium (μ/L)	Vanadium (μ/L)	Zinc (μ/L)	Mercury (μ/L)
Laboratory			TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA	TA
TW-22 (duplicate)	Downgradient	4/24/2008	<1,000	<60	336	<50	<15	<25	744,000	<50	<50	<100	6,470	<50	1,680,000	1,220	70.9 J	<200	403,000	48.7 J	<50	14,100,000	<50	<50	<150	0.12 J
		4/24/2008	<1,000	<60	347	<50	<15	<25	813,000	<50	<50	<100	6,990	<50	1,910,000	1,420	72.9 J	<200	422,000	<1,000	<50	15,500,000	<50	135	<150	<0.20
TW-23	Downgradient	4/24/2008	326 J	<60	448	22 J	<15	<25	854,000	<50	<50	<100	13,900	<50	2,260,000	1,770	56 J	<200	502,000	<1,000	<50	17,100,000	<50	<50	<150	<0.20
TW-24	Downgradient	4/22/2008	341 J	<60	171	<50	<15	<25	782,000	<50	<50	<100	<500	<50	2,130,000	357	281	<200	608,000	108 J	<50	16,500,000	<50	135	<150	<0.20
TW-25	Upgradient	4/22/2008	1,620	<60	174	32.8 J	<15	<25	671,000	<50	<50	<100	1,170	<50	1,810,000	54	320	<200	590,000	83.9 J	<50	14,200,000	<75	200	<150	<0.20
TW-26	Crossgradient	4/22/2008	<1,000	<60	206	<50	<15	<25	673,000	<50	<50	<100	681	<50	1,760,000	321	267	<200	506,000	<1,000	<50	14,500,000	<75	91	<150	<0.20
TW-27	Crossgradient	4/22/2008	1,230	<60	473	46	<15	<25	782,000	<50	<50	<100	13,400	<50	2,070,000	1,120	110	<200	487,000	<1,000	<50	15,600,000	<50	10.7 J	<150	<0.20
TW-28	Within Injection Zone	4/22/2008	510 J	<60	573	28.3 J	<15	<25	731,000	<50	<50	<100	5,850	<50	1,880,000	1,320	<100	<200	448,000	<1,000	<50	14,400,000	<50	<50	<150	<0.20
TW-29	Downgradient	4/22/2008	597 J	<60	454	29.7 J	<15	<25	776,000	<50	<50	25.2 J	22,900	<50	2,100,000	1,290	<100	<200	424,000	<1,000	<50	14,700,000	<50	<50	<150	<0.20
IW-02	Injection Well	4/24/2008	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA
IW-03	Injection Well	4/24/2008	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA

^{a/} μg/L = micrograms per liter.
^{b/} M-flag indicates Recovery/RPD poor for MS/MSD.
^{c/} J-flag indicates the concentration is above the method detection limit but below the laboratory reporting limit, the concentration is estimated.

CSIA Data

Altus Sites OU-1 and SS-17

TABLE 3
SUMMARY OF CARBON STABLE ISOTOPE ANALYSIS
OU-1 BIOWALL DEMONSTRATION
ALTUS AFB, OKLAHOMA

Sample Identification	Location Description	Analysis (units)	Sample Date	TCE	<i>cis</i> -1,2-DCE	<i>trans</i> -1,2-DCE	VC	Ethene
EPAUMP1	Within Biowall	USEPA Laboratory VOCs (µg)	6-Sep-07	550	91.8	3.47	7.7	NA
		VOCs with CSIA (µg/L)	6-Sep-07	1,000	100	6.0	10	0.025
		Carbon Fractionization (‰)	6-Sep-07	-25.99	-27.81	NR	NR	NR
MP1	Within Biowall	USEPA Laboratory VOCs (µg)	6-Sep-07	0.21 J	5.27	9.49	53.4	NA
		VOCs with CSIA (µg/L)	6-Sep-07	0.9 J	7.0	20	200	0.32
		Carbon Fractionization (‰)	6-Sep-07	NR	-0.36	-22.21	-11.94	NR
MP4	30' Downgradient	USEPA Laboratory VOCs (µg)	6-Sep-07	58.4	186	31.1	82.6	NA
		VOCs with CSIA (µg/L)	6-Sep-07	90	300	60	200	0.69
		Carbon Fractionization (‰)	6-Sep-07	-23.55	-22.94	-29.10	-21.41	NR

J = the reported value is an estimated concentration

NA = not analyzed

NR = value cannot be calculated due to concentrations less than detection.

TABLE 3
SUMMARY OF CARBON STABLE ISOTOPE ANALYSIS
SS-17 FULL-SCALE BIOWALL
ALTUS AFB, OKLAHOMA

Sample Identification	Location Description	Analysis (units)	Sample Date	TCE	<i>cis</i> -1,2-DCE	<i>trans</i> -1,2-DCE	VC	Ethene
BB04U	30' Upgradient	USEPA Laboratory VOCs (µg/L)	6-Sep-07	3,930	79.5	9.53	1.92	NA
		VOCs with CSIA (µg/L)	6-Sep-07	7,000	100	20	4.0 J	0.10
		Carbon Fractionization (‰)	6-Sep-07	-23.68	-22.59	NR	NR	NR
BB04W	Within Biowall	USEPA Laboratory VOCs (µg/L)	6-Sep-07	1.45	2.55	<1.0	0.52	NA
		VOCs with CSIA (µg/L)	6-Sep-07	3.0 J	4.0 J	0.6 J	6.0	0.21
		Carbon Fractionization (‰)	6-Sep-07	NR	-11.95	NR	NR	NR
BB04D	30' Downgradient	USEPA Laboratory VOCs (µg/L)	6-Sep-07	3,150	187	5.98	56.5	NA
		VOCs with CSIA (µg/L)	6-Sep-07	6,000	300	10	100	1.0
		Carbon Fractionization (‰)	6-Sep-07	-23.68	-22.59	NR	NR	NR
BB05U	30' Upgradient	USEPA Laboratory VOCs (µg/L)	6-Sep-07	154	288	12.6	0.88	NA
		VOCs with CSIA (µg/L)	6-Sep-07	300	400	20	2.0 J	0.009 J
		Carbon Fractionization (‰)	6-Sep-07	-22.00	-22.22	NR	NR	NR
BB05W	Within Biowall	USEPA Laboratory VOCs (µg/L)	6-Sep-07	2.54	5.04	0.28 J	1.15	NA
		VOCs with CSIA (µg/L)	6-Sep-07	5.0 J	7.0	0.5 J	2.0 J	0.17
		Carbon Fractionization (‰)	6-Sep-07	NR	-23.68	NR	NR	NR
BB05D	30' Downgradient	USEPA Laboratory VOCs (µg/L)	6-Sep-07	376	79.9	3.31	18.4	NA
		VOCs with CSIA (µg/L)	6-Sep-07	700	90	6.0	40	0.16
		Carbon Fractionization (‰)	6-Sep-07	-22.52	-23.2	NR	-21.36	NR

J = the reported value is an estimated concentration

NA = not analyzed

NR = value cannot be calculated due to concentrations less than detection.

Dover AFB

TABLE 7
SUMMARY OF CARBON STABLE ISOTOPE ANALYSIS
SITE WP-14 BIOWALL DEMONSTRATION
DOVER AFB, DELAWARE

Sample Location	Location Description	Sample Date	Analysis (units) ^{a/}	Date Analyzed	TCE ^{b/}	cis -1,2-DCE ^{b/}	VC ^{b/}	Ethene
North Transect Monitoring Wells								
TS-MW11	5' Upgradient of East Biowall	3/18/2008	Laboratory VOCs (µg/L)	24-Mar-08	1.7	3.1	<1.0	0.17
			VOCs with CSIA (µg/L)	29-Mar-08	2.0 J	4.0 J	<5.0	0.17
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-25.85	-23.15	NR	NR
TS-MW11D (duplicate)	5' Upgradient of East Biowall	3/18/2008	Laboratory VOCs (µg/L)	24-Mar-08	1.6	3.2	<1.0	0.04
			VOCs with CSIA (µg/L)	29-Mar-08	2.0 J	4.0 J	0.6 J	0.04
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-26.19	-23.56	NR	NR
TS-MW01	Within First (East) Biowall	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	3.8	23	0.064 J	0.078
			VOCs with CSIA (µg/L)	29-Mar-08	1.0 J	9.0	0.8 J	0.078
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-25.88	-20.82	NR	NR
TS-MW02	Between Biowalls	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	1.7	9.6	1.7	0.10
			VOCs with CSIA (µg/L)	29-Mar-08	3.0 J	20	1.0 J	0.10
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-26.22	-26.88	NR	NR
TS-MW03	Within Second (West) Biowall	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	3.1	7.9	<1.0	0.12
			VOCs with CSIA (µg/L)	29-Mar-08	2.0 J	10	2.0 J	0.12
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-25.43	-21.01	NR	NR
TS-MW04	15' Downgradient of West Biowall	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	12	19	12	0.33
			VOCs with CSIA (µg/L)	29-Mar-08	3.0 J	8.0	<5.0	0.33
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-26.08	-24.57	NR	NR
South Transect Monitoring Wells (Amended with Sulfate)								
TS-MW12	10' Upgradient of East Biowall	3/18/2008	Laboratory VOCs (µg/L)	24-Mar-08	0.29 J	<1.0	<1.0	0.022J
			VOCs with CSIA (µg/L)	29-Mar-08	0.3 J	1.0 J	<5.0	0.022 J
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	NR	NR	NR	NR
TS-MW06	Within First (East) Biowall	3/18/2005	Laboratory VOCs (µg/L)	24-Mar-08	0.93 J	1.6	0.88 J	0.12
			VOCs with CSIA (µg/L)	29-Mar-08	<5.0	2.0 J	<5.0	0.12
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	NR	NR	NR	NR
TS-MW07	Between Biowalls	3/20/2008	Laboratory VOCs (µg/L)	24-Mar-08	9.8	86	80	0.79
			VOCs with CSIA (µg/L)	3-Apr-08	10	20	20	0.79
			Carbon Fractionization- δ ¹³ C (‰)	31-Jul-08	-36.51	-28.55	-25.00	NR
TS-MW08	Within Second (West) Biowall	3/20/2008	Laboratory VOCs (µg/L)	28-Mar-08	10	94	82	2.0
			VOCs with CSIA (µg/L)	3-Apr-08	9.0	80	50	2.0
			Carbon Fractionization- δ ¹³ C (‰)	31-Jul-08	-27.00	-25.89	-20.49	NR
TS-MW09	15' Downgradient of West Biowall	3/17/2008	Laboratory VOCs (µg/L)	24-Mar-08	4.5	7.9	<1.0	0.04
			VOCs with CSIA (µg/L)	29-Mar-08	4.0 J	10	4.0 J	0.04
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-33.04	-28.41	NR	NR

^{a/} µg/L = micrograms per liter; ‰ = parts per thousand or "per mil."

^{b/} TCE = trichloroethene, DCE = dichloroethene, VC = vinyl chloride.

^{c/} NA = not analyzed

Seneca Depot

TABLE 3
SUMMARY OF CARBON STABLE ISOTOPE ANALYSIS
ASH LANDFILL BIOWALL, SENECA ARMY DEPOT ACTIVITY, NEW YORK

Sample Identification	Location Description	Analysis (units)	Sample Date	TCE	cis-1,2-DCE	VC	Ethene
MWT-25	upgradient of Biowall A	Laboratory VOCs (µg/L)	15-Nov-07	26	17	0.64 J	NA
		VOCs with CSIA (µg/L)	10-Jan-08	3.0 J	1.0 J	<5.0	0.033
		Carbon Fractionization (‰)	10-Jan-08	-21.32	NR	NR	NR
TEMP-1	In Biowall A	Laboratory VOCs (µg/L)	10-Jan-08	3.6	53	24	11
		VOCs with CSIA (µg/L)	10-Jan-08	4.0 J	50	30	12
		Carbon Fractionization (‰)	10-Jan-08	-19.38	-15.26	-21.13	NR
MWT-26	upgradient of Biowalls B1/B2	Laboratory VOCs (µg/L)	15-Nov-07	2.8	2.8	<1.0	0.40
		VOCs with CSIA (µg/L)	10-Jan-08	2.0 J	1.0 J	<5.0	0.016 J
		Carbon Fractionization (‰)	10-Jan-08	NR	NR	NR	NR
MWT-27	in Biowall B1	Laboratory VOCs (µg/L)	15-Nov-07	<10	<10	<10	0.014 J
		VOCs with CSIA (µg/L)	9-Jan-08	<5.0	0.3 J	<5.0	0.077
		Carbon Fractionization (‰)	9-Jan-08	NR	NR	NR	NR
MWT-28	in Biowall B2	Laboratory VOCs (µg/L)	15-Nov-07	<5.0	<5.0	<5.0	ND
		VOCs with CSIA (µg/L)	9-Jan-08	0.3 J	0.4 J	<5.0	0.023 J
		Carbon Fractionization (‰)	9-Jan-08	NR	NR	NR	NR
MWT-29	downgradient of Biowall B2	Laboratory VOCs (µg/L)	14-Nov-07	4.4	96	74	200
		VOCs with CSIA (µg/L)	9-Jan-08	6.0	70	60	17
		Carbon Fractionization (‰)	9-Jan-08	-15.87	-13.51	-20.28	NR
MWT-22	downgradient of Biowall B2	Laboratory VOCs (µg/L)	14-Nov-07	2.6	99	180	NA
		VOCs with CSIA (µg/L)	10-Jan-08	1.0 J	40	90	120
		Carbon Fractionization (‰)	10-Jan-08	NR	0.41	-5.6	-21.88
PT-22	between Biowalls B and C	Laboratory VOCs (µg/L)	14-Nov-07	9.7	30	11	NA
		VOCs with CSIA (µg/L)	10-Jan-08	<5.0	0.8	<5.0	0.39
		Carbon Fractionization (‰)	10-Jan-08	NR	NR	NR	NR
MWT-36	Duplicate of MWT-26	Laboratory VOCs (µg/L)	15-Nov-07	2.8	2.8	<1.0	0.40
		VOCs with CSIA (µg/L)	10-Jan-08	2.0 J	1.0 J	<5.0	0.019 J
		Carbon Fractionization (‰)	10-Jan-08	NR	NR	NR	NR

J = the reported value is an estimated concentration

NA = not analyzed

NR = value cannot be calculated due to concentrations less than detection.

Dugway PG

TABLE 8
SUMMARY OF CARBON STABLE ISOTOPE ANALYSIS
SWMU-97 PILOT TEST, DUGWAY PROVING GROUND, UTAH

Sample Location	Sample Identification	Location Description	Analysis (units) ^{a/}	Sample Date	Date Analyzed	TCE ^{b/}	cis -1,2-DCE ^{b/}	VC ^{b/}	Ethene
TW22	097GW082(TW22)	Downgradient	Laboratory VOCs (µg/L)	24-Apr-08	25-Apr-08	2300	6.1 J	<50	NA ^{c/}
			VOCs with CSIA (µg/L)	24-Apr-08	6-May-08	1,000	3.0 J	<5.0	1.5
			Carbon Fractionization- δ ¹³ C (‰)	24-Apr-08	1-Aug-08	-17.87	-31.08	NR ^{d/}	NR
TW22	097FD082(TW22) (Field Duplicate)	Downgradient	Laboratory VOCs (µg/L)	24-Apr-08	25-Apr-08	1300	<50	<50	NA
			VOCs with CSIA (µg/L)	24-Apr-08	6-May-08	1000	3.0 J	<5.0	1.5
			Carbon Fractionization- δ ¹³ C (‰)	24-Apr-08	1-Aug-08	-18.10	-30.28	NR	NR
TW23	097GW083(TW23)	Downgradient	Laboratory VOCs (µg/L)	24-Apr-08	25-Apr-08	660	<50	<50	NA
			VOCs with CSIA (µg/L)	24-Apr-08	6-May-08	650	<100	<100	1.3
			Carbon Fractionization- δ ¹³ C (‰)	24-Apr-08	1-Aug-08	-17.04	NR	NR	NR
TW24	097GW084(TW24)	Downgradient	Laboratory VOCs (µg/L)	22-Apr-08	23-Apr-08	1300	<20	<20	NA
			VOCs with CSIA (µg/L)	22-Apr-08	2-May-08	1000	<5.0	<5.0	0.44
			Carbon Fractionization- δ ¹³ C (‰)	22-Apr-08	31-Jul-08	-18.15	NR	NR	NR
TW25	097GW085(TW25)	Upgradient	Laboratory VOCs (µg/L)	23-Apr-08	25-Apr-08	1400	<50	<50	NA
			VOCs with CSIA (µg/L)	23-Apr-08	2-May-08	1000	0.3 J	<5.0	1.5
			Carbon Fractionization- δ ¹³ C (‰)	23-Apr-08	31-Jul-08	-17.86	NR	NR	NR
TW28	097GW088(TW28)	Injection Area	Laboratory VOCs (µg/L)	23-Apr-08	25-Apr-08	1500	<100	<100	NA
			VOCs with CSIA (µg/L)	23-Apr-08	2-May-08	1000	3.0 J	0.7 J	1.4
			Carbon Fractionization- δ ¹³ C (‰)	23-Apr-08	1-Aug-08	-17.73	NR	NR	NR
TW29	097GW089(TW29)	Down/Crossgradient	Laboratory VOCs (µg/L)	23-Apr-08	25-Apr-08	1800	<50	<50	NA
			VOCs with CSIA (µg/L)	23-Apr-08	2-May-08	1000	2.0 J	<5.0	1.2
			Carbon Fractionization- δ ¹³ C (‰)	23-Apr-08	1-Aug-08	-18.28	-40.49	NR	NR
IW02	097GW090(IW02)	Injection Well	Laboratory VOCs (µg/L)	24-Apr-08	25-Apr-08	<50	<50	<50	NA
			VOCs with CSIA (µg/L)	24-Apr-08	6-May-08	24	3.2 J	<5.0	0.47
			Carbon Fractionization- δ ¹³ C (‰)	24-Apr-08	1-Aug-08	-19.71	-55.55	NR	NR
IW03	097GW091(IW03)	Injection Well	Laboratory VOCs (µg/L)	24-Apr-08	25-Apr-08	<20	<20	<20	NA
			VOCs with CSIA (µg/L)	24-Apr-08	6-May-08	7.2	<5.0	<5.0	0.56
			Carbon Fractionization- δ ¹³ C (‰)	24-Apr-08	1-Aug-08	-27.99	-39.74	NR	NR

^{a/} µg/L = micrograms per liter; ‰ = parts per thousand or "per mil."

^{b/} TCE = trichloroethene, DCE = dichloroethene, VC = vinyl chloride.

^{c/} NA = not analyzed

^{d/} NR = value cannot be calculated due to limit in concentrations.

^{e/} J = the reported value is an estimated concentration

Appendix C
PHREEQC Modeling Output and Supporting Materials

Geochemical Equilibrium Modeling

A geochemical model, PHREEQC (Parkhurst and Appelo, 1999), was used to evaluate the saturation state of the reduced iron phases that may be present in the biowalls. PHREEQC is a thermodynamic equilibrium program designed to model chemical speciation in aqueous solutions, determine the saturation states of solutions with minerals and gases, and predict the results of various reactions, such as dissolution of minerals and oxidation.

The modeling will show which reduced iron phases or minerals are saturated (if any) for each solution. Generally, if a solution is at saturation with respect to a mineral, that mineral would be expected to be present within the material in which the water is in contact (i.e. the biowall). Minerals which are undersaturated would dissolve when placed in contact with the solution, while minerals that are supersaturated would eventually precipitate the material (assuming the mineral forms at low temperature).

PHREEQC uses a term called the saturation index (SI) to quantify the degree of saturation of a mineral. SI is defined as follows:

$$SI = \text{Log} (IAP/K_{sp})$$

Where IAP is the ion activity product and K_{sp} is the solubility product constant for the phase in question. For phases at saturation, $IAP=K_{sp}$ and $SI = 0$. A negative SI indicates that the phase is undersaturated ($IAP<K_{sp}$) while a positive SI ($IAP>K_{sp}$) indicates the phase is supersaturated. In practice, a range of 0 ± 0.5 SI units is considered saturated due to uncertainties in analytical and thermodynamic data.

Water Analyses Internal Consistency Evaluation

The analyses were checked for internal consistency using both charge balance and mass balance relationships. The charge balance was calculated as follows:

$$\frac{(\sum(\text{Cations} \times \text{charge}) - \sum(\text{Anions} \times \text{charge}))}{(\sum(\text{Cations} \times \text{charge}) + \sum(\text{Anions} \times \text{charge}))} \times 100\%$$

Where “cations” refers to the molar concentration of positively charged ions (moles/L) and “anions” to the molar concentration of negatively charged ions.

The mass balance was calculated using the following relationship:

$$(\text{TDS-Calc} - \text{TDS-Meas})/\text{TDS-Meas} \times 100\%$$

TDS was calculated by summing the concentrations of all species in mg/L. Adjustments were made in cases where the species that would be formed upon evaporation was in a different form than that provided by the laboratory. For instance, silicon reported as “Si” (atomic mass = 28.09 g/mole) was converted to “SiO₂” (atomic mass = 60.09 g/mole) using the factor 2.14 (60.09g/mole / 28.09 g/mole = 2.14). In addition, the bicarbonate

concentration was multiplied by a factor of 0.49 to account for loss of carbon dioxide gas during evaporation.

By evaluating both the mass balance and charge balance, conclusions could be drawn about the accuracy and completeness of the analysis. The possible mass balance and charge balance combinations and the corresponding interpretations are shown in **Table 1**.

Table 1 - Interpretation of Charge and Mass Balance Results

Mass Balance	Charge Balance	Interpretation ¹
Positive	Positive	Cations are over-reported
Positive	Negative	Anions are over-reported
Negative	Negative	Cations are under-reported and/or one or more important cations were not analyzed
Negative	Positive	Anions are under-reported and/or one or more important anions were not analyzed

1. Note that the interpretation represents the least complex explanation. In some cases, multiple problems with an analysis may have caused the inconsistencies.

A summary of the analyses used for each site and the adjustments made to the data are provided in **Tables 2a through 2e**.

Table 2a - Summary of Water Samples Used for PHREEQC Geochemical Modeling - EPA Column Experiment.

Sample ID	Date Sampled	Notes
Column B3E	5-15-07	The 5-15-07 dataset was the only date in which sufficient parameters were analyzed to allow the modeling to be performed. Only alkalinity was missing, and this was estimated to achieve a reasonable charge and mass balance. A value of 840 mg/L alkalinity (as bicarbonate) was used in the model (689 mg/L as CaCO ₃).

The total alkalinity value used for May 2007 (689 mg/L) is slightly lower than the range of values measured between May 2006 and February 2007 (790 - 1,080 mg/L). However, given the apparent decreasing alkalinity trend over the course of the experiment, 689 mg/L is a reasonable value.

Table 2b - Summary of Water Samples Used for PHREEQC Geochemical Modeling - Altus Air Force Base.

Sample ID	Date Sampled	Notes
BB04U	9-6-07	Alkalinity of 4,200 mg/L resulted in a charge balance (CB) of -37% and a mass balance (MB) of +58%. Alkalinity (as bicarbonate) was adjusted to 550 mg/L.
BB04W	9-6-07	Alkalinity of 12,600 mg/L resulted in a CB of -62% and a MB of +147%. Alkalinity was adjusted to 1,500 mg/L.
BB04D	9-6-07	Alkalinity of 6,400 mg/L resulted in a CB of -44% and a MB of +77%. Alkalinity was adjusted to 950 mg/L.
BB05U	9-6-07	Alkalinity of 5,600 mg/L resulted in a CB of -50% and a MB of +91%. Alkalinity was adjusted to 950 mg/L.
BB05W	9-6-07	Alkalinity of 1,806 mg/L resulted in a CB of -0.1% and a MB of +4.5%. Alkalinity was not modified.
BB05D	9-6-07	Alkalinity of 9,200 mg/L resulted in a CB of -63% and a MB of +187%. Alkalinity was adjusted to 850 mg/L.
EPAUMP1	9-6-07	Alkalinity of 2,900 mg/L resulted in a CB of -32% and a MB of +55%. Alkalinity was adjusted to 240 mg/L.
MP1	9-6-07	Alkalinity of 15,600 mg/L resulted in a CB of -77% and a MB of +366%. Alkalinity was adjusted to 2,000 mg/L.
MP2	9-6-07	Alkalinity of 17,400 mg/L resulted in a CB of -69% and a MB of +232%. Alkalinity was adjusted to 2,200 mg/L.
MP3	9-6-07	Alkalinity of 98,000 mg/L resulted in a CB of -94% and a MB of +1678%. Alkalinity was adjusted to 1,100 mg/L.
MP4	9-6-07	Alkalinity of 98,000 mg/L resulted in a CB of -94% and a MB of +1354%. Alkalinity was adjusted to 1,400 mg/L.

The alkalinity measurements for the Altus samples are extremely high and resulted in very poor mass and charge balance. In addition, analyses from the same well for different dates vary by 1-2 orders of magnitude. For instance, for well MP4, an alkalinity of 960 mg/L was reported for April 11, 2007, while a value of 95,000 was reported for September 6, 2007. Note that the charge balance- and mass balance-adjusted value or 1,400 mg/L bicarbonate alkalinity (1,148 mg/L total alkalinity) is reasonably close to the 960 mg/L total alkalinity measured in April 2007 for well MP4.

Table 2c - Summary of Water Samples Used for PHREEQC Geochemical Modeling - Seneca Army Depot.

Sample ID	Date Sampled	Notes
MWT-25	1-10-08	Alkalinity was not analyzed. Set bicarbonate alkalinity to 510 mg/L. No temperature data were collected. Assumed 25°C for modeling purposes.
TEMP-1	1-10-08	No temperature data were collected. Assumed 25°C for modeling purposes.
MWT-26	1-10-08	Alkalinity was not analyzed. Set bicarbonate alkalinity to 0 mg/L. No temperature data were collected. Assumed 25°C for modeling purposes.
MWT-27	1-9-08	Alkalinity was not analyzed. Set bicarbonate alkalinity to 1,950 mg/L. No temperature data were collected. Assumed 25°C for modeling purposes.
MWT-28	1-9-08	Alkalinity was not analyzed. Set bicarbonate alkalinity to 850 mg/L. No temperature data were collected. Assumed 25°C for modeling purposes.
MWT-29	1-9-08	Alkalinity was not analyzed. Set bicarbonate alkalinity to 490 mg/L. No temperature data were collected. Assumed 25°C for modeling purposes.
MWT-22	1-10-08	Alkalinity was not analyzed. Set bicarbonate alkalinity to 1,320 mg/L. No temperature data were collected. Assumed 25°C for modeling purposes.
PT-22	1-10-08	Alkalinity was not analyzed. Set bicarbonate alkalinity to 330 mg/L. No temperature data were collected. Assumed 25°C for modeling purposes.

Alkalinity was not measured for the Seneca Army Depot samples. Therefore, the alkalinity was estimated based on charge balance and mass balance, as shown in **Table 2c**. In addition, no temperature data were reported, so a value of 25°C was used in the model. The error associated with the temperature is not expected to be important, as the PHREEQC database does not have enthalpy data for many of the phases of concern anyway, which does not allow temperature corrections to be made.

Table 2d – Summary of Water Samples Used for PHREEQC Geochemical Modeling – Dover Air Force Base.

Sample ID	Date Sampled	Notes
TS-MW11	3-18-08	No changes or additions to data
TS-MW01	3-18-08	Alkalinity of 1,050 mg/L resulted in a CB of -52% and a MB of +128%. Alkalinity was adjusted to 365 mg/L.
TS-MW02	3-19-08	No changes or additions to data
TS-MW03	3-19-08	Alkalinity of 1,100 mg/L resulted in a CB of -34% and a MB of +64%. Alkalinity was adjusted to 647 mg/L.
TS-MW04	3-19-08	No changes or additions to data
TS-MW12	3-18-08	No changes or additions to data
TS-MW06	3-18-08	No changes or additions to data
TS-MW07	3-20-08	No changes or additions to data
TS-MW08	3-28-08	No changes or additions to data
TS-MW09	3-17-08	No changes or additions to data

The Dover AFB data were, in general, internally consistent, with the exception of samples TS-MW01 and TS-MW03, in which the alkalinity required adjustment.

Table 2e – Summary of Water Samples Used for PHREEQC Geochemical Modeling – Dugway Proving Ground.

Sample ID	Date Sampled	Notes
TW-22	4-24-08	No changes or additions to data
TW-23	4-24-08	No changes or additions to data
TW-24	4-22-08	No changes or additions to data
TW-25	4-22-08	No changes or additions to data
TW-26	4-22-08	TDS was not measured, so a mass balance could not be performed.
TW-27	4-22-08	No changes or additions to data
TW-28	4-22-08	No changes or additions to data
TW-29	4-22-08	No changes or additions to data

The Dugway data were internally consist, although for two of the samples, TDS was not measured, so a mass balance could not be performed.

A summary of the mass and charge balances following the necessary corrections is provided in Appendix B.

PHREEQC Thermodynamic Database

The thermodynamic database used by PHREEQC was supplemented to include the iron phases that have been proposed as chlorinated solvent reducing agents as well as other iron phases of interest. The phases that were added and the thermodynamic data used are shown in **Table 3**.

Table 3 - Summary of Thermodynamic Data Added to the PHREEQC Database

Phase	Reaction	Log Ksp	ΔH° (kcal)
Troilite	$\text{Fe}^{2+}(\text{aq}) + \text{S}^{2-}(\text{aq}) \rightarrow \text{FeS}(\text{s})$	19.08	-10.89
Pyrite	$\text{Fe}^{2+}(\text{aq}) + \text{S}^0(\text{aq}) + \text{S}^{2-}(\text{aq}) \rightarrow \text{FeS}_2(\text{s})$	29.26	-27.59
Marcasite	$\text{Fe}^{2+}(\text{aq}) + \text{S}^0(\text{aq}) + \text{S}^{2-}(\text{aq}) \rightarrow \text{FeS}_2(\text{s})$	28.57	-26.59
Mackinawite	$\text{Fe}^{2+}(\text{aq}) + \text{S}^{2-}(\text{aq}) \rightarrow \text{FeS}(\text{s})$	17.56	-8.49
Greigite	$\text{Fe}^{2+}(\text{aq}) + 2\text{Fe}^{3+}(\text{aq}) + 4\text{S}^{2-}(\text{aq}) \rightarrow \text{Fe}_3\text{S}_4(\text{s})$	90.44	-57.37
Amorphous Iron Monosulfide	$\text{Fe}^{2+}(\text{aq}) + \text{S}^{2-}(\text{aq}) \rightarrow \text{FeS}(\text{amorphous})$	16.83	-7.49
Ferrous Hydroxide1	$\text{Fe}^{2+}(\text{aq}) + 2\text{H}_2\text{O}(\text{l}) \rightarrow \text{Fe}(\text{OH})_2(\text{s}) + 2\text{H}^+(\text{aq})$	-13.89	-
Ferrous Hydroxide2	$\text{Fe}^{2+}(\text{aq}) + 2\text{H}_2\text{O}(\text{l}) \rightarrow \text{Fe}(\text{OH})_2(\text{s}) + 2\text{H}^+(\text{aq})$	-12.94	-
Ferrous Oxide	$\text{Fe}^{2+}(\text{aq}) + \text{H}_2\text{O}(\text{l}) \rightarrow \text{FeO}(\text{s}) + 2\text{H}^+(\text{aq})$	-13.59	-
Hydroxycarbonate Green Rust (GR)	$6\text{Fe}^{2+}(\text{aq}) + \text{CO}_3^{2-}(\text{aq}) + 12\text{H}_2\text{O} \rightarrow [\text{Fe}^{+2}_4\text{Fe}^{+3}_2(\text{OH})_{12}][\text{CO}_3](\text{s}) + 12\text{H}^+(\text{aq}) + 2\text{e}^-$	-58.35	-
Hydroxysulfate GR	$6\text{Fe}^{2+}(\text{aq}) + \text{SO}_4^{2-}(\text{aq}) + 12\text{H}_2\text{O}(\text{l}) \rightarrow [\text{Fe}^{+2}_4\text{Fe}^{+3}_2(\text{OH})_{12}][\text{SO}_4](\text{s}) + 12\text{H}^+(\text{aq}) + 2\text{e}^-$	-60.38	-
Hydroxychloride GR	$4\text{Fe}^{2+}(\text{aq}) + \text{Cl}^- + 8\text{H}_2\text{O} \rightarrow [\text{Fe}^{+2}_3\text{Fe}^{+3}(\text{OH})_8][\text{Cl}](\text{s}) + 8\text{H}^+(\text{aq}) + \text{e}^-$	-43.56	-
Hydroxy GR	$3\text{Fe}^{2+}(\text{aq}) + 7\text{H}_2\text{O}(\text{l}) \rightarrow [\text{Fe}^{+2}_2\text{Fe}^{+3}(\text{OH})_7](\text{s}) + 7\text{H}^+(\text{aq}) + \text{e}^-$	-24.99	-
Hydroxy GR	$2\text{Fe}^{2+}(\text{aq}) + 5\text{H}_2\text{O}(\text{l}) \rightarrow [\text{Fe}^{+2}\text{Fe}^{+3}(\text{OH})_5](\text{s}) + 5\text{H}^+(\text{aq}) + \text{e}^-$	-23.09	-
Hydroxy GR	$3\text{Fe}^{2+}(\text{aq}) + 8\text{H}_2\text{O}(\text{l}) \rightarrow [\text{Fe}^{+2}_2\text{Fe}^{+3}(\text{OH})_7](\text{s}) + 8\text{H}^+(\text{aq}) + 2\text{e}^-$	-42.12	-
Magnetite	$3\text{Fe}^{2+}(\text{aq}) + 4\text{H}_2\text{O}(\text{l}) \rightarrow \text{Fe}_3\text{O}_4(\text{s}) + 8\text{H}^+(\text{aq}) + 2\text{e}^-$	-45.80	-
Lepidocrocite	$\text{Fe}^{2+}(\text{aq}) + 2\text{H}_2\text{O}(\text{l}) \rightarrow \gamma\text{-FeOOH}(\text{s}) + 3\text{H}^+(\text{aq}) + \text{e}^-$	-16.67	-

A more detailed presentation of the thermodynamic data, including the data sources and calculations performed is included in Appendix B.

Oxidation-Reduction Potential

Results

Reaction	Standard Potential - E^0 (volts)
$\text{S}^0(\text{aq}) + 2\text{e}^- \rightarrow \text{S}^{2-}(\text{aq})$	-0.508
$\text{H}_2\text{SO}_3(\text{aq}) + 4\text{H}^+ + 4\text{e}^- \rightarrow \text{S}^0(\text{aq}) + 3\text{H}_2\text{O}(\text{l})$	+0.450
$\text{SO}_4^{2-}(\text{aq}) + 4\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2\text{SO}_3(\text{aq}) + \text{H}_2\text{O}(\text{l})$	+0.200
$\text{SO}_4^{2-}(\text{aq}) + 8\text{H}^+ + 8\text{e}^- \rightarrow \text{S}^{2-}(\text{aq}) + 4\text{H}_2\text{O}(\text{l})$	+0.142

$$Eh(\text{volts}) = E^0(\text{volts}) + (2.3RT/nF) \log ([\text{SO}_4^{2-}][\text{H}^+]^8 / [\text{S}^{2-}])$$

Where

R (gas constant)	= 0.001987 kcal/K-mol
K (Faraday constant)	= 23.06 kcal/volt
E^0 (standard potential)	= +0.142 volts
n (number of e- in reaction)	= 8

The equation is then simplified to:

$$Eh \text{ (volts)} = 0.142 + 0.0074 \log ([SO_4^{2-}][H^+]^8/[S^{2-}])$$

The square bracketed terms refer to the activities of each species, which were determined by the PHREEQC program prior to calculating the Eh.

References

Parkhurst, D.L. and Appelo, C.A.J. 1999. User's Guide to PHREEQC (Version 2)- A Computer Program for Speciation, Batch-Reaction, One-Dimensional Transport, and Inverse Geochemical Calculations. USGS Water-Resources Investigations Report 99-4259.

Weast, R. C. and M. J. Astle. 1982. *Handbook of Chemistry and Physics*. 62nd Ed, 1981-82. CRC Press, Inc. Boca Raton, Florida.

Mass and Charge Balance

Original Data

	ANALYSES (mg/L)																						CHG IMASS BAL		
Site	Sample	Ba ⁺²	Ca ⁺²	Mg ⁺²	Na ⁺	K ⁺	Fe ⁺²	Mn ⁺²	DOC	SiO ₂	SO ₄ ⁻²	S ⁻²	Cl ⁻	NO ₃ ⁻	CO3	NO ₂ ⁻	HCO ₃ ⁻	TDS (Calc)	TDS (Meas)	Cations (millimoles)	Anions (millimoles)	AB Diff	CB% Diff	MB % Diff	Conclusion
Dover	TS-MW11	0	3.4	2.1	11	0.78	1	0.03	3	0	19.2		9.4	0	0		22.81	61	83	0.9	1.0	-0.2	-8.3	-26.4	Missing cations
Dover	TS-MW01	0	49	22	14	9.2	45	0.59	16	0	3.5		12	0			1281	799	350	6.7	21.4	-14.7	-52.1	128.3	Too many anions
Dover	TS-MW02	0	14	8.1	15	2.4	1.5	0.1	5	0	15		9.7	0			102.5	121	210	2.1	2.3	-0.1	-2.9	-42.4	Missing cations
Dover	TS-MW03	0	120	30	14	19	1.9	40	33	0	7.5		12	0			1342	935	570	11.1	22.5	-11.4	-34.0	64.0	Too many anions
Dover	TS-MW04	0	10	6.4	12	1	0.01	0.14	2.5	0	9.2		9.8	0			85.4	93	120	1.6	1.9	-0.3	-8.3	-22.6	Missing cations
Dover	TS-MW12	0	7.4	4.9	8	1.2	0.01	0.12	1.5	0	34		6.5	0.32			21.96	75	110	1.2	1.3	-0.1	-4.1	-32.1	Missing cations
Dover	TS-MW6	0	180	27	9.3	1.8	2.5	0.3	2.8	0	530		6.5	0.57			434.3	974	680	11.8	18.3	-6.6	-21.8	43.2	Too many anions
Dover	TS-MW7	0	470	37	12	1.8	1.32	2.5	5.3	0	970		7.9	0			475.8	1741	1900	27.2	28.2	-1.0	-1.8	-8.4	Missing cations
Dover	TS-MW8	0	1200	83	16	43	0.27	1.8	63	0	1000		0.5	0.23			780.8	2790	4500	68.7	33.6	35.1	34.3	-38.0	Missing anions
Dover	TS-MW9	0	93	53	13	1.6	1.82	1.2	5.9	0	430		7.1	0.65			3.416	609	690	9.7	9.2	0.5	2.7	-11.7	Missing anions
Altus	BB04U	0.01	339	156	777	5.06	0.2	0.16	2.28	16.8	1780		623	1.86			5124	6212	3940	63.7	138.6	-74.9	-37.0	57.7	Too many anions
Altus	BB04W	0.18	328	154	960	17.8	0.01	0.02	10.6	28.3	1220		804	0.55			15372	11056	4480	71.3	300.0	-228.8	-61.6	146.8	Too many anions
Altus	BB04D	0.01	365	168	893	8.88	0.25	0.65	5.5	19.4	1690		770	0.15			7808	7747	4380	71.2	184.9	-113.7	-44.4	76.9	Too many anions
Altus	BB05U	0.01	227	161	625	2.75	0.1	0.01	2.28	23.8	1560		419	0.12			6832	6369	3340	51.9	156.3	-104.4	-50.2	90.7	Too many anions
Altus	BB05W	0.24	351	167	1110	18.3	0.01	0.1	10.4	31.7	1290		839	0.5	0		1806	4703	4500	80.0	80.1	-0.1	-0.1	4.5	Too many anions
Altus	BB05D	0.03	237	146	606	3.53	0.75	0.83	5.12	23.8	1040		465	0	0		11224	8028	2800	50.4	218.7	-168.4	-62.6	186.7	Too many anions
Altus	EPAUMP1	0.01	530	129	445	5.78	0.51	0.11	0	15.6	2040		336	0			3538	5236	3380	56.6	109.9	-53.3	-32.0	54.9	Too many anions
Altus	MP1	0.72	366	114	334	25.9	1.94	1.6	0	38.1	145		267	0			19032	10620	2280	43.0	322.5	-279.5	-76.5	365.8	Too many anions
Altus	MP2	0.22	779	141	418	58.1	0.19	0.94	0	40.7	1220		283	0			21228	13343	4020	70.3	381.3	-311.1	-68.9	231.9	Too many anions
Altus	MP3	0.02	595	138	427	12.3	3.07	1.13	0	24.4	1480		267	0			119560	61532	3460	60.1	1997.9	-1937.8	-94.2	1678.4	Too many anions
Altus	MP4	0.01	596	135	474	7.12	3.95	1.2	0	20.9	1870		309	0			115900	60208	4140	61.9	1947.3	-1885.4	-93.8	1354.3	Too many anions
Seneca	MWT-25	0	160	33	48	13	0.06	0.36	0	0	190	1.3	33	1.2	0	0.25	0	479	730	13.1	4.9	8.2	45.7	-34.4	Missing anions
Seneca	TEMP-1	0	170	18	24	4.3	13	8.5	13	0	180	1.9	29	0.5	0	0.93	475.8	693	690	11.9	12.4	-0.5	-1.9	0.5	Too many anions
Seneca	MWT-26	0	230	49	120	26	0.04	0.01	6.1	0	1000	1	55	1.4	0	0.25	0	1488	1400	21.4	22.4	-1.0	-2.2	6.3	Too many anions
Seneca	MWT-27	0	430	80	50	94	66	7.2	167	0	10	0.6	40	0.98	0	0.25	0	945	1900	35.3	1.4	33.9	92.6	-50.3	Missing anions
Seneca	MWT-28	0	230	32	16	34	27	3.7	92	0	3.1	1.6	9.2	1	0	1.1	0	448	820	16.8	0.3	16.5	96.0	-45.4	Missing anions
Seneca	MWT-29	0	160	29	44	13	0.1	0.9	20.9	0	220	1	18	1.3	0	0.41	0	507	750	12.7	5.1	7.6	42.5	-32.4	Missing anions
Seneca	MWT-22	0	310	52	110	8.3	3.5	5.7	0	0	100	1.6	47	1	0	0.25	0	638	1300	25.1	3.4	21.7	76.0	-51.0	Missing anions
Seneca	PT-22	0	130	36	29	9.2	0.3	0.1	0	0	170	1.6	130	0.99	0	1.5	0	506	670	11.0	7.2	3.7	20.6	-24.5	Missing anions
Dugway	TW-22	0	850	2000	15000	550	6.1	1.22	9.3	0	11600		27100	0	0	0	745.4	57482	59000	873.8	1018.2	-144.4	-7.6	-2.6	Missing cations
Dugway	TW-23	0	860	2300	16000	690	11	1.77	100	0	11200		29600	0	0	0	1569	61532	63000	946.3	1093.9	-147.6	-7.2	-2.3	Missing cations
Dugway	TW-24	0	770	2000	18000	660	0.04	0.36	9.5	0	11600		29800	0	0	0	303.8	62989	60000	1002.9	1087.1	-84.2	-4.0	5.0	Too many anions
Dugway	TW-25	0	760	2200	17000	740	0.09	0.05	8.6	0	12400		24700	0	0	0	377	57993	57000	977.4	961.1	16.3	0.8	1.7	Too many cations
Dugway	TW-26	0	760	2000	17000	650	0.67	0.32	8.9	0	11900		26800	0	0	0	301.3	59268	0	958.7	1008.7	-50.1	-2.5		
Dugway	TW-27	0	800	2400	18000	520	8.6	1.12	198	0	10900		25600	0	0	0	1934	59375	0	1034.1	980.8	53.3	2.6		
Dugway	TW-28	0	740	1900	16000	530	4.1	1.32	121	0	10400		24700	0	0	0	2856	55796	54000	903.0	960.1	-57.1	-3.1	3.3	Too many anions
Dugway	TW-29	0	760	2200	16000	500	18	1.29	228	0	10800		25900	0	0	0	2313	57541	56000	928.4	993.4	-65.0	-3.4	2.8	Too many anions
Dugway	IW-02	0	890	2100	14000	580	38	0	3390	0	8040		24800	0	0	0	2291	54961	59000	842.4	904.6	-62.1	-3.6	-6.8	Missing cations
Dugway	IW-03	0	1200	2200	13000	690	47	0	4420	0	9270		24500	0	0	0	2583	56593	62000	825.8	926.5	-100.7	-5.7	-8.7	Missing cations
Col B3	5/15/07	0.16	436	183	790	9.31	0.04	0	5.39	0	1670	7.55	812	0	0	0	0	3906	4680	71	57.7	13.8	10.7	-16.5	Missing anions

Adjusted Data

ANALYSES (mg/L)																		CHG IMASS BAL							
Site	Sample	Ba ⁺²	Ca ⁺²	Mg ⁺²	Na ⁺	K ⁺	Fe ⁺²	Mn ⁺²	DOC	SiO ₂	SO ₄ ⁻²	S ⁻²	Cl ⁻	NO ₃ ⁻	CO3	NO ₂ ⁻	HCO ₃ ⁻	TDS	TDS	Cations	Anions	AB	CB%	MB%	Conclusion
																		(Calc)	(Meas)	(millimoles)	(millimoles)	Diff	Diff	Diff	
Dover	TS-MW11	0	3.4	2.1	11	0.78	1	0.03	3	0	19.2		9.4	0	0		22.81	61	83	0.9	1.0	-0.2	-8.3	-26.4	Missing cations
Dover	TS-MW01	0	49	22	14	9.2	45	0.59	16	0	3.5		12	0			365	350	350	6.7	6.4	0.3	2.6	0.0	Too many cations
Dover	TS-MW02	0	14	8.1	15	2.4	1.5	0.1	5	0	15		9.7	0			102.5	121	210	2.1	2.3	-0.1	-2.9	-42.4	Missing cations
Dover	TS-MW03	0	120	30	14	19	1.9	40	33	0	7.5		12	0			647	594	570	11.1	11.1	0.0	-0.1	4.3	Too many anions
Dover	TS-MW04	0	10	6.4	12	1	0.01	0.14	2.5	0	9.2		9.8	0			85.4	93	120	1.6	1.9	-0.3	-8.3	-22.6	Missing cations
Dover	TS-MW12	0	7.4	4.9	8	1.2	0.01	0.12	1.5	0	34		6.5	0.32			21.96	75	110	1.2	1.3	-0.1	-4.1	-32.1	Missing cations
Dover	TS-MW6	0	180	27	9.3	1.8	2.5	0.3	2.8	0	530		6.5	0.57			434.3	974	680	11.8	18.3	-6.6	-21.8	43.2	Too many anions
Dover	TS-MW7	0	470	37	12	1.8	1.32	2.5	5.3	0	970		7.9	0			475.8	1741	1900	27.2	28.2	-1.0	-1.8	-8.4	Missing cations
Dover	TS-MW8	0	1200	83	16	43	0.27	1.8	63	0	1000		0.5	0.23			780.8	2790	4500	68.7	33.6	35.1	34.3	-38.0	Missing anions
Dover	TS-MW9	0	93	53	13	1.6	1.82	1.2	5.9	0	430		7.1	0.65			3.416	609	690	9.7	9.2	0.5	2.7	-11.7	Missing anions
Altus	BB04U	0.01	339	156	777	5.06	0.2	0.16	2.28	16.8	1780		623	1.86			550	3971	3940	63.7	63.7	0.0	0.0	0.8	Too many cations
Altus	BB04W	0.18	328	154	960	17.8	0.01	0.02	10.6	28.2857143	1220		804	0.55			1500	4258	4480	71.3	72.7	-1.4	-1.0	-4.9	Missing cations
Altus	BB04D	0.01	365	168	893	8.88	0.25	0.65	5.5	19.3928571	1690		770	0.15			950	4386	4380	71.2	72.5	-1.3	-0.9	0.1	Too many anions
Altus	BB05U	0.01	227	161	625	2.75	0.1	0.01	2.28	23.7857143	1560		419	0.12			650	3340	3340	51.9	55.0	-3.1	-2.9	0.0	Missing cations
Altus	BB05W	0.24	351	167	1110	18.3	0.01	0.1	10.4	31.7142857	1290		839	0.5	0		1806	4703	4500	80.0	80.1	-0.1	-0.1	4.5	Too many anions
Altus	BB05D	0.03	237	146	606	3.53	0.75	0.83	5.12	23.7857143	1040		465	0	0		850	2945	2800	50.4	48.7	1.7	1.7	5.2	Too many cations
Altus	EPAUMP1	0.01	530	129	445	5.78	0.51	0.11	0	15.6428571	2040		336	0			240	3620	3380	56.6	55.9	0.7	0.7	7.1	Too many cations
Altus	MP1	0.72	366	114	334	25.9	1.94	1.6	0	38.1428571	145		267	0			2000	2274	2280	43.0	43.3	-0.3	-0.4	-0.2	Missing cations
Altus	MP2	0.22	779	141	418	58.1	0.19	0.94	0	40.7142857	1220		283	0			2200	4019	4020	70.3	69.4	0.8	0.6	0.0	Missing anions
Altus	MP3	0.02	595	138	427	12.3	3.07	1.13	0	24.4285714	1480		267	0			1100	3487	3460	60.1	56.4	3.8	3.2	0.8	Too many cations
Altus	MP4	0.01	596	135	474	7.12	3.95	1.2	0	20.8714286	1870		309	0			1400	4103	4140	61.9	70.6	-8.7	-6.6	-0.9	Missing cations
Seneca	MWT-25	0	160	33	48	13	0.06	0.36	0	0	190	1.3	33	1.2	0	0.25	510	729	730	13.1	13.3	-0.1	-0.4	-0.2	Missing cations
Seneca	TEMP-1	0	170	18	24	4.3	13	8.5	13	0	180	1.9	29	0.5	0	0.93	475.8	693	690	11.9	12.4	-0.5	-1.9	0.5	Too many anions
Seneca	MWT-26	0	230	49	120	26	0.04	0.01	6.1	0	1000	1	55	1.4	0	0.25	0	1488	1400	21.4	22.4	-1.0	-2.2	6.3	Too many anions
Seneca	MWT-27	0	430	80	50	94	66	7.2	167	0	10	0.6	40	0.98	0	0.25	1950	1901	1900	35.3	33.3	2.0	2.9	0.0	Too many cations
Seneca	MWT-28	0	230	32	16	34	27	3.7	92	0	3.1	1.6	9.2	1	0	1.1	850	865	820	16.8	14.3	2.5	8.1	5.4	Too many cations
Seneca	MWT-29	0	160	29	44	13	0.1	0.9	20.9	0	220	1	18	1.3	0	0.41	490	747	750	12.7	13.1	-0.5	-1.8	-0.4	Missing cations
Seneca	MWT-22	0	310	52	110	8.3	3.5	5.7	0	0	100	1.6	47	1	0	0.25	1320	1284	1300	25.1	25.1	0.0	0.1	-1.2	Missing anions
Seneca	PT-22	0	130	36	29	9.2	0.3	0.1	0	0	170	1.6	130	0.99	0	1.5	330	667	670	11.0	12.6	-1.7	-7.0	-0.4	Missing cations
Dugway	TW-22	0	850	2000	15000	550	6.1	1.22	9.3	0	11600		27100	0	0	0	745.4	57482	59000	873.8	1018.2	-144.4	-7.6	-2.6	Missing cations
Dugway	TW-23	0	860	2300	16000	690	11	1.77	100	0	11200		29600	0	0	0	1569	61532	63000	946.3	1093.9	-147.6	-7.2	-2.3	Missing cations
Dugway	TW-24	0	770	2000	18000	660	0.04	0.36	9.5	0	11600		29800	0	0	0	303.8	62989	60000	1002.9	1087.1	-84.2	-4.0	5.0	Too many anions
Dugway	TW-25	0	760	2200	17000	740	0.09	0.05	8.6	0	12400		24700	0	0	0	377	57993	57000	977.4	961.1	16.3	0.8	1.7	Too many cations
Dugway	TW-26	0	760	2000	17000	650	0.67	0.32	8.9	0	11900		26800	0	0	0	301.3	59268	0	958.7	1008.7	-50.1	-2.5		
Dugway	TW-27	0	800	2400	18000	520	8.6	1.12	198	0	10900		25600	0	0	0	1934	59375	0	1034.1	980.8	53.3	2.6		
Dugway	TW-28	0	740	1900	16000	530	4.1	1.32	121	0	10400		24700	0	0	0	2856	55796	54000	903.0	960.1	-57.1	-3.1	3.3	Too many anions
Dugway	TW-29	0	760	2200	16000	500	18	1.29	228	0	10800		25900	0	0	0	2313	57541	56000	928.4	993.4	-65.0	-3.4	2.8	Too many anions
Dugway	IW-02	0	890	2100	14000	580	38	0	3390	0	8040		24800	0	0	0	2291	54961	59000	842.4	904.6	-62.1	-3.6	-6.8	Missing cations
Dugway	IW-03	0	1200	2200	13000	690	47	0	4420	0	9270		24500	0	0	0	2583	56593	62000	825.8	926.5	-100.7	-5.7	-8.7	Missing cations
Col B3	5/15/07	0.16	436	183	790	9.31	0.04	0	5.39	0	1670	7.55	812	0	0	0	840	4318	4680	71	71.4	0.0	0.0	-7.7	Missing anions

Thermodynamic Data

Phase	Formula	ΔG_f° (kcal)	ΔH_f° (kcal)	S° (ca/mol-K)	C_p° (ca/mol-K)	Reaction	ΔG_r° (kcal)	Log Ksp	ΔH_r° (kcal)	
Troilite	FeS (s)	-24.37	-24.3	14.42		12.07 Fe^{2+} (aq) + S^{2-} (aq) \rightarrow FeS (troilite)	-26.03	19.08	-10.8918	Anderko and Shur, 1997
Pyrite	FeS ₂ (s)	-38.26	-41	12.65		14.85 Fe^{2+} (aq) + S^0 (aq) + S^{2-} (aq) \rightarrow FeS ₂ (pyrite)	-39.92	29.26	-27.5918	
Marcasite	FeS ₂ (s)	-37.32	-40	12.87		14.91 Fe^{2+} (aq) + S^0 (aq) + S^{2-} (aq) \rightarrow FeS ₂ (marcasite)	-38.98	28.57	-26.5918	
Mackinawite	FeS (s)	-22.3	-21.9	15.4		12 Fe^{2+} (aq) + S^{2-} (aq) \rightarrow FeS (mackinawite)	-23.96	17.56	-8.49	
Greigite	Fe ₃ S ₄ (s)	-69.4	-70.3	47.1		42 Fe^{2+} (aq) + 2 Fe^{3+} (aq) + 4 S^{2-} (aq) \rightarrow Fe ₃ S ₄ (greigite)	-123.38	90.44	-57.37	
Amorphous Iron Monosulfide	FeS (s)	-21.3	-20.9	15.4		12 Fe^{2+} (aq) + S^{2-} (aq) \rightarrow FeS (amorphous)	-22.96	16.83	-7.49	
FeHS ⁺ (aq)	FeHS ⁺ (aq)	-24.93	-36.5	-9		29.6 Fe^{2+} (aq) + HS ⁻ (aq) \rightarrow FeS (mackinawite) + H ⁺	-3.5			Rickard, 2006
Fe ²⁺ (aq)	Fe ²⁺ (aq)	-18.9	-21.3							
Fe ³⁺ (aq)	Fe ³⁺ (aq)	-4.6	-11.6							
S ²⁻ (aq)	S ²⁻ (aq)	20.5	7.9	-3.5						
S ⁰ (aq)	S ⁰ (aq)	0	0	7.6						

Phase	Formula	ΔG_f° (kcal)	Reaction	ΔG_r° (kcal)	Log K
Ferrous Hydroxide1	Fe(OH) ₂	-116.3	Fe ⁺² + 2H ₂ O → Fe(OH) ₂ (s) + 2H ⁺	18.95	-13.89
Ferrous Hydroxide	Fe(OH) ₂	-117.1	Fe ⁺² + 2H ₂ O → Fe(OH) ₂ (s) + 2H ⁺	18.14	-13.29
Ferrous Hydroxide2	Fe(OH) ₂	-117.6	Fe ⁺² + 2H ₂ O → Fe(OH) ₂ (s) + 2H ⁺	17.66	-12.94
Ferrous Oxide	FeO	-60.0	Fe ⁺² + H ₂ O → FeO (s) + 2H ⁺	18.54	-13.59
Hydroxycarbonate GR	[Fe+24Fe+32 (OH)12][CO3·2H2O]	-966.25	6Fe ⁺² + CO ₃ ⁻² + 14H ₂ O → [Fe+24Fe+32 (OH)12][CO3·2H2O] (s) + 12H ⁺ + 2e ⁻	84.76	-62.13
Hydroxycarbonate GR	[Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][CO ₃]	-858.031	6Fe ⁺² + CO ₃ ⁻² + 12H ₂ O → [Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][CO ₃] (s) + 12H ⁺ + 2e ⁻	79.60	-58.35
Hydroxycarbonate GR	[Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][CO ₃]	-925.43	6Fe ⁺² + CO ₃ ⁻² + 12H ₂ O → [Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][CO ₃] (s) + 12H ⁺ + 2e ⁻	12.20	-8.95
Hydroxysulfate GR	[Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][SO ₄]	-907.027	6Fe ⁺² + SO ₄ ⁻² + 12H ₂ O → [Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][SO ₄] (s) + 12H ⁺ + 2e ⁻	82.38	-60.38
Hydroxysulfate GR	[Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][SO ₄]	-905.832	6Fe ⁺² + SO ₄ ⁻² + 12H ₂ O → [Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][SO ₄] (s) + 12H ⁺ + 2e ⁻	83.57	-61.26
Hydroxysulfate GR	[Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][SO ₄ ·8H ₂ O]	-909.895	6Fe ⁺² + SO ₄ ⁻² + 20H ₂ O → [Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][SO ₄ ·8H ₂ O] (s) + 12H ⁺	533.0	-390.71
Hydroxysulfite GR	[Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][SO ₃ ·4H ₂ O]	-1233.75	6Fe ⁺² + SO ₃ ⁻² + 16H ₂ O → [Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂][SO ₃ ·4H ₂ O] (s) + 12H ⁺ + 2e ⁻	-79.2	58.08
Hydroxychloride GR	[Fe ⁺² ₃ Fe ⁺³ (OH) ₈][Cl]	-512.906	4Fe ⁺² + Cl ⁻ + 8H ₂ O → [Fe ⁺² ₃ Fe ⁺³ (OH) ₈][Cl] (s) + 8H ⁺ + e ⁻	59.4	-43.56
Hydroxychloride GR	[Fe ⁺² ₃ Fe ⁺³ (OH) ₈][Cl·2H ₂ O]	-509.56	4Fe ⁺² + Cl ⁻ + 10H ₂ O → [Fe ⁺² ₃ Fe ⁺³ (OH) ₈][Cl·2H ₂ O] (s) + 8H ⁺ + e ⁻	176.1	-129.12
Hydroxy GR	[Fe+22Fe+3 (OH)7]	-430.139	3Fe ⁺² + 7H ₂ O → [Fe+22Fe+3 (OH)7] (s) + 7H ⁺ + e ⁻	32.3	-24.99
Hydroxy GR	[Fe+2Fe+3 (OH)5]	-297.347	2Fe ⁺² + 5H ₂ O → [Fe+2Fe+3 (OH)5] (s) + 5H ⁺ + e ⁻	29.8	-23.09
Hydroxy GR	[Fe+32Fe+2 (OH)8]	-464.699	3Fe ⁺² + 8H ₂ O → [Fe+22Fe+3 (OH)7] (s) + 8H ⁺ + 2e ⁻	54.4	-42.12
Magnetite	Fe ₃ O ₄	-242.017	3Fe ⁺² + 4H ₂ O → Fe ₃ O ₄ + 8H ⁺ + 2e ⁻	50.3	-45.8
Magnetite	Fe ₃ O ₄	-242.017	3Fe ⁺² + 4H ₂ O → Fe ₃ O ₄ + 8H ⁺ + 2e ⁻	50.3	-45.8
Lepidocrocite	γ-FeOOH	-112.5	Fe ⁺² + 2H ₂ O → γ-FeOOH + 3H ⁺ + e ⁻	22.7	-16.7

Species	ΔG_f° (kcal)	ΔH_f° (kcal)	Source	Notes:
H ₂ O(l)	-56.69		CRC, 1989 ¹ ; NBS, 1952 ¹	
H ₂ O(l)	-56.69		Bard et al., 1985 ³ ; Kelsall and Williams, 1991 ³ .	
CO ₃ ⁻²	-126.17		CRC, 1989 ¹	1. Cited in Drissi et al., 1995, Table 4.
CO ₃ ⁻²	-126.17		Wagman, 1982 ²	
HCO ₃ ⁻	-140.26		CRC, 1989 ¹	2. Cited in Genin et al., 1998.
HCO ₃ ⁻	-140.25		Wagman, 1982 ²	3. Cited in Refait, 1999.
H ₂ CO ₃ ⁰	-148.94		CRC, 1989 ¹	4. Cited in Stumm and Morgan, 1981
H ₂ CO ₃ ⁰	-148.95		Wagman, 1982 ²	
Fe ⁺²	-20.3		NBS, 1952 ¹	
Fe ⁺²	-21.9		Kelsall and Williams, 1991 ²	
Fe ⁺²	-21.9		Yang, 1982	
FeOH ⁺	-66.3		NBS, 1973 ¹	
FeOH ⁺	-66.3		Kelsall and Williams, 1991 ²	
Fe ³⁺ (aq)	-4.6		Stumm and Morgan, 1981	
FeOOH ⁻	-90.63		NBS, 1952 ¹	
FeOOH ⁻	-89.96		Kelsall and Williams, 1991 ²	
Fe(OH) ₂ ⁺	-106.2		NBS, 1952 ¹	
Fe(OH) ₂ ⁺	-104.685		Wagman, 1982 ²	
Cl ⁻	-31.3576		Wagman, 1982 ²	
SO ₄ ⁻²	-177.94		Wagman, 1982 ²	
SO ₄ ⁻²	-177.95		Bard et al., 1985 ³ ; Kelsall and Williams, 1991 ³ .	
SO ₃ ⁻²	-116.3		NBS, 1973 ⁴	

PHREEQC Model Output

Altus Sites OU-1 and SS-17

Input file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\Altus.pqi
Output file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\Altus.pqi
Database file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\phreeqc8.dat

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\phreeqc8.dat

SOLUTION 1 BB04U 9-6-2007

temp	22.1
pH	6.89
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
N	1.86
Fe	0.2
S(6)	1780 as SO4
S(-2)	0.005
Cl	623
Br	3.34
Alkalinity	550 as HCO3
Ba	0.01
Ca	339
Mg	156
Na	777
K	5.06
Mn	0.16
Si	7.84
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. BB04U 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	9.014e-003	9.014e-003
Ba	7.281e-008	7.281e-008
Br	4.180e-005	4.180e-005
Ca	8.458e-003	8.458e-003
Cl	1.757e-002	1.757e-002
Fe	3.581e-006	3.581e-006
K	1.294e-004	1.294e-004
Mg	6.417e-003	6.417e-003
Mn	2.912e-006	2.912e-006
N	1.328e-004	1.328e-004
Na	3.380e-002	3.380e-002
S(-2)	1.559e-007	1.559e-007
S(6)	1.853e-002	1.853e-002
Si	1.305e-004	1.305e-004

-----Description of solution-----

pH	=	6.890
pe	=	4.000
Activity of water	=	0.998
Ionic strength	=	7.612e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	1.101e-002
Total CO2 (mol/kg)	=	1.101e-002
Temperature (deg C)	=	22.100
Electrical balance (eq)	=	1.025e-005
Percent error, 100*(Cat- An)/(Cat+ An)	=	0.01
Iterations	=	13
Total H	=	1.110220e+002
Total O	=	5.561187e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.8732	-0.1683

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.538e-007	1.288e-007	-6.813	-6.890	-0.077
OH-	7.930e-008	6.210e-008	-7.101	-7.207	-0.106
H2O	5.551e+001	9.985e-001	1.744	-0.001	0.000
Ba	7.281e-008				
BaSO4	3.736e-008	3.802e-008	-7.428	-7.420	0.008
Ba+2	3.438e-008	1.416e-008	-7.464	-7.849	-0.385
BaHCO3+	1.056e-009	8.429e-010	-8.976	-9.074	-0.098

BaCO3	1.581e-011	1.609e-011	-10.801	-10.794	0.008
BaOH+	4.661e-015	3.719e-015	-14.332	-14.430	-0.098
Br	4.180e-005				
Br-	4.180e-005	3.245e-005	-4.379	-4.489	-0.110
C (4)	1.101e-002				
HCO3-	8.446e-003	6.803e-003	-2.073	-2.167	-0.094
CO2	2.015e-003	2.050e-003	-2.696	-2.688	0.008
CaHCO3+	2.494e-004	2.009e-004	-3.603	-3.697	-0.094
MgHCO3+	1.793e-004	1.431e-004	-3.746	-3.844	-0.098
NaHCO3	9.871e-005	1.005e-004	-4.006	-3.998	0.008
CaCO3	8.832e-006	8.988e-006	-5.054	-5.046	0.008
CO3-2	5.537e-006	2.331e-006	-5.257	-5.633	-0.376
MgCO3	3.803e-006	3.870e-006	-5.420	-5.412	0.008
NaCO3-	1.232e-006	9.831e-007	-5.909	-6.007	-0.098
FeHCO3+	7.391e-007	5.898e-007	-6.131	-6.229	-0.098
MnHCO3+	5.266e-007	4.202e-007	-6.279	-6.377	-0.098
MnCO3	1.261e-007	1.283e-007	-6.899	-6.892	0.008
FeCO3	4.762e-008	4.847e-008	-7.322	-7.315	0.008
Fe (CO3) (OH) -	1.831e-009	1.461e-009	-8.737	-8.835	-0.098
BaHCO3+	1.056e-009	8.429e-010	-8.976	-9.074	-0.098
Fe (CO3) 2-2	3.273e-010	1.327e-010	-9.485	-9.877	-0.392
BaCO3	1.581e-011	1.609e-011	-10.801	-10.794	0.008
Ca	8.458e-003				
Ca+2	5.721e-003	2.426e-003	-2.243	-2.615	-0.373
CaSO4	2.479e-003	2.523e-003	-2.606	-2.598	0.008
CaHCO3+	2.494e-004	2.009e-004	-3.603	-3.697	-0.094
CaCO3	8.832e-006	8.988e-006	-5.054	-5.046	0.008
CaOH+	3.910e-009	3.120e-009	-8.408	-8.506	-0.098
CaHSO4+	2.304e-009	1.838e-009	-8.638	-8.736	-0.098
Cl	1.757e-002				
Cl-	1.757e-002	1.380e-002	-1.755	-1.860	-0.105
MnCl+	4.881e-008	3.895e-008	-7.311	-7.409	-0.098
FeCl+	2.069e-008	1.651e-008	-7.684	-7.782	-0.098
MnCl2	2.305e-010	2.346e-010	-9.637	-9.630	0.008
MnCl3-	1.117e-012	8.914e-013	-11.952	-12.050	-0.098
FeCl+2	8.844e-023	3.586e-023	-22.053	-22.445	-0.392
FeCl2+	3.039e-024	2.425e-024	-23.517	-23.615	-0.098
FeCl3	3.287e-027	3.345e-027	-26.483	-26.476	0.008
Fe (2)	3.581e-006				
Fe+2	1.998e-006	8.669e-007	-5.699	-6.062	-0.363
FeSO4	7.692e-007	7.828e-007	-6.114	-6.106	0.008
FeHCO3+	7.391e-007	5.898e-007	-6.131	-6.229	-0.098
FeCO3	4.762e-008	4.847e-008	-7.322	-7.315	0.008
FeCl+	2.069e-008	1.651e-008	-7.684	-7.782	-0.098
FeS	2.572e-009	2.618e-009	-8.590	-8.582	0.008
FeOH+	2.139e-009	1.707e-009	-8.670	-8.768	-0.098
Fe (CO3) (OH) -	1.831e-009	1.461e-009	-8.737	-8.835	-0.098
Fe (CO3) 2-2	3.273e-010	1.327e-010	-9.485	-9.877	-0.392
Fe (HS) 2	2.886e-012	2.937e-012	-11.540	-11.532	0.008
FeHSO4+	8.233e-013	6.569e-013	-12.084	-12.182	-0.098
Fe (OH) 2	1.256e-013	1.278e-013	-12.901	-12.893	0.008
Fe (HS) 3-	2.471e-017	1.972e-017	-16.607	-16.705	-0.098
Fe (3)	1.941e-014				
Fe (OH) 2+	1.145e-014	9.134e-015	-13.941	-14.039	-0.098

Fe (OH) 3	7.888e-015	8.027e-015	-14.103	-14.095	0.008
Fe (OH) 4-	6.321e-017	5.044e-017	-16.199	-16.297	-0.098
FeOH+2	9.810e-018	3.977e-018	-17.008	-17.400	-0.392
FeSO4+	6.515e-021	5.198e-021	-20.186	-20.284	-0.098
Fe (SO4) 2-	7.548e-022	6.023e-022	-21.122	-21.220	-0.098
Fe+3	4.665e-022	9.443e-023	-21.331	-22.025	-0.694
FeCl+2	8.844e-023	3.586e-023	-22.053	-22.445	-0.392
FeCl2+	3.039e-024	2.425e-024	-23.517	-23.615	-0.098
FeHSO4+2	4.433e-027	1.797e-027	-26.353	-26.745	-0.392
FeCl3	3.287e-027	3.345e-027	-26.483	-26.476	0.008
Fe2 (OH) 2+4	1.778e-032	4.805e-034	-31.750	-33.318	-1.568
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-42.470	-44.920	-2.451
H (0)	1.326e-011				
H2	6.628e-012	6.746e-012	-11.179	-11.171	0.008
K	1.294e-004				
K+	1.250e-004	9.814e-005	-3.903	-4.008	-0.105
KSO4-	4.399e-006	3.510e-006	-5.357	-5.455	-0.098
KOH	2.592e-012	2.638e-012	-11.586	-11.579	0.008
Mg	6.417e-003				
Mg+2	4.152e-003	1.819e-003	-2.382	-2.740	-0.358
MgSO4	2.082e-003	2.119e-003	-2.682	-2.674	0.008
MgHCO3+	1.793e-004	1.431e-004	-3.746	-3.844	-0.098
MgCO3	3.803e-006	3.870e-006	-5.420	-5.412	0.008
MgOH+	2.125e-008	1.696e-008	-7.673	-7.771	-0.098
Mn (2)	2.912e-006				
Mn+2	1.597e-006	6.930e-007	-5.797	-6.159	-0.363
MnSO4	6.135e-007	6.243e-007	-6.212	-6.205	0.008
MnHCO3+	5.266e-007	4.202e-007	-6.279	-6.377	-0.098
MnCO3	1.261e-007	1.283e-007	-6.899	-6.892	0.008
MnCl+	4.881e-008	3.895e-008	-7.311	-7.409	-0.098
MnCl2	2.305e-010	2.346e-010	-9.637	-9.630	0.008
MnOH+	1.363e-010	1.087e-010	-9.866	-9.964	-0.098
MnCl3-	1.117e-012	8.914e-013	-11.952	-12.050	-0.098
Mn (NO3) 2	0.000e+000	0.000e+000	-165.142	-165.134	0.008
Mn (3)	1.426e-034				
Mn+3	1.426e-034	1.870e-035	-33.846	-34.728	-0.882
N (-3)	7.333e-006				
NH4+	6.859e-006	5.275e-006	-5.164	-5.278	-0.114
NH4SO4-	4.562e-007	3.640e-007	-6.341	-6.439	-0.098
NH3	1.864e-008	1.897e-008	-7.730	-7.722	0.008
N (0)	1.255e-004				
N2	6.273e-005	6.384e-005	-4.203	-4.195	0.008
N (3)	0.000e+000				
NO2-	0.000e+000	0.000e+000	-58.827	-58.937	-0.110
N (5)	0.000e+000				
NO3-	0.000e+000	0.000e+000	-79.679	-79.789	-0.110
Mn (NO3) 2	0.000e+000	0.000e+000	-165.142	-165.134	0.008
Na	3.380e-002				
Na+	3.283e-002	2.626e-002	-1.484	-1.581	-0.097
NaSO4-	8.673e-004	6.921e-004	-3.062	-3.160	-0.098
NaHCO3	9.871e-005	1.005e-004	-4.006	-3.998	0.008
NaCO3-	1.232e-006	9.831e-007	-5.909	-6.007	-0.098
NaOH	1.321e-009	1.345e-009	-8.879	-8.871	0.008
O (0)	0.000e+000				

O2		0.000e+000	0.000e+000	-70.992	-70.984	0.008
S (-2)	1.559e-007					
HS-		7.874e-008	6.166e-008	-7.104	-7.210	-0.106
H2S		7.462e-008	7.594e-008	-7.127	-7.120	0.008
FeS		2.572e-009	2.618e-009	-8.590	-8.582	0.008
Fe (HS) 2		2.886e-012	2.937e-012	-11.540	-11.532	0.008
S-2		1.148e-013	4.730e-014	-12.940	-13.325	-0.385
Fe (HS) 3-		2.471e-017	1.972e-017	-16.607	-16.705	-0.098
S (6)	1.853e-002					
SO4-2		1.309e-002	5.357e-003	-1.883	-2.271	-0.388
CaSO4		2.479e-003	2.523e-003	-2.606	-2.598	0.008
MgSO4		2.082e-003	2.119e-003	-2.682	-2.674	0.008
NaSO4-		8.673e-004	6.921e-004	-3.062	-3.160	-0.098
KSO4-		4.399e-006	3.510e-006	-5.357	-5.455	-0.098
FeSO4		7.692e-007	7.828e-007	-6.114	-6.106	0.008
MnSO4		6.135e-007	6.243e-007	-6.212	-6.205	0.008
NH4SO4-		4.562e-007	3.640e-007	-6.341	-6.439	-0.098
HSO4-		7.899e-008	6.303e-008	-7.102	-7.200	-0.098
BaSO4		3.736e-008	3.802e-008	-7.428	-7.420	0.008
CaHSO4+		2.304e-009	1.838e-009	-8.638	-8.736	-0.098
FeHSO4+		8.233e-013	6.569e-013	-12.084	-12.182	-0.098
FeSO4+		6.515e-021	5.198e-021	-20.186	-20.284	-0.098
Fe (SO4) 2-		7.548e-022	6.023e-022	-21.122	-21.220	-0.098
FeHSO4+2		4.433e-027	1.797e-027	-26.353	-26.745	-0.392
Si	1.305e-004					
H4SiO4		1.303e-004	1.326e-004	-3.885	-3.877	0.008
H3SiO4-		1.716e-007	1.370e-007	-6.765	-6.863	-0.098
H2SiO4-2		1.472e-013	5.968e-014	-12.832	-13.224	-0.392

-----Saturation indices-----

Phase	SI		log IAP	log KT	
[Fe2(OH) 5]	-3.64	19.45	23.09	Fe2(OH) 5	
[Fe3(OH) 7]	2.18	27.17	24.99	Fe3(OH) 7	
[Fe3(OH) 8]	-10.94	31.18	42.12	Fe3(OH) 8	
[Fe6(OH) 12] [CO3]	-23.43	34.92	58.35	Fe6(OH) 12 (CO3) 1	
[Fe6(OH) 12] [SO4]	-22.10	38.28	60.38	Fe6(OH) 12 (SO4) 1	
[Fe6(OH) 8] [Cl]	-17.43	26.13	43.56	Fe4(OH) 8 (Cl) 1	
Anhydrite	-0.54	-4.89	-4.35	CaSO4	
Aragonite	0.07	-8.25	-8.32	CaCO3	
Barite	-0.10	-10.12	-10.02	BaSO4	
Brucite	-5.75	11.04	16.79	Mg (OH) 2	
Calcite	0.22	-8.25	-8.46	CaCO3	
Chalcedony	-0.29	-3.88	-3.59	SiO2	
Chrysotile	-7.20	25.36	32.56	Mg3Si2O5 (OH) 4	
CO2 (g)	-1.26	-2.69	-1.43	CO2	
Dolomite	0.40	-16.62	-17.02	CaMg (CO3) 2	
Epsomite	-2.86	-5.02	-2.16	MgSO4:7H2O	
Fe (OH) 2 (1)	-5.22	7.72	12.94	Fe (OH) 2	
Fe (OH) 2 (2)	-6.17	7.72	13.89	Fe (OH) 2	
Fe (OH) 3 (a)	-6.25	-1.36	4.89	Fe (OH) 3	
FeO	-5.87	7.72	13.59	FeO	
FeS (am)	-2.50	-6.38	-3.88	FeS	

FeS (ppt)	-2.47	-6.38	-3.92	FeS
Goethite	-0.46	-1.36	-0.90	FeOOH
Greigite	-12.69	-51.39	-38.71	Fe3S4
Gypsum	-0.31	-4.89	-4.58	CaSO4:2H2O
H2 (g)	-8.03	-11.17	-3.14	H2
H2O (g)	-1.59	-0.00	1.59	H2O
H2S (g)	-6.16	-7.12	-0.96	H2S
Halite	-5.02	-3.44	1.58	NaCl
Hausmannite	-30.86	30.89	61.75	Mn3O4
Hematite	1.07	-2.71	-3.79	Fe2O3
Jarosite-H3O	-24.46	-36.17	-11.71	H3OFe3 (SO4) 2 (OH) 6
Jarosite-K	-22.37	-33.29	-10.92	KFe3 (SO4) 2 (OH) 6
Lepidocrocite	-4.97	11.73	16.70	FeOOH
Lime	-11.65	11.16	22.81	Ca (OH) 2
Mackinawite	-1.77	-6.38	-4.62	FeS
Mackinawite(2)	-2.90	0.60	3.50	FeS
Magnetite	-14.62	31.18	45.80	Fe3O4
Manganite	-13.70	11.64	25.34	MnOOH
Marcasite	5.39	-12.45	-17.84	FeS2
Melanterite	-6.09	-8.34	-2.24	FeSO4:7H2O
N2 (g)	-0.94	-4.19	-3.25	N2
Nesquehonite	-2.80	-8.37	-5.58	MgCO3:3H2O
NH3 (g)	-9.55	-7.72	1.83	NH3
O2 (g)	-68.04	-70.98	-2.95	O2
Pyrite	6.11	-12.45	-18.56	FeS2
Pyrochroite	-7.58	7.62	15.20	Mn (OH) 2
Pyrolusite	-26.20	15.65	41.85	MnO2
Quartz	0.15	-3.88	-4.02	SiO2
Rhodochrosite	-0.67	-11.79	-11.12	MnCO3
Schwertmannite(1)	-50.24	-39.74	10.50	Fe8O8 (OH) 4.4 (SO4) 1.8:8.4H2O
Schwertmannite(2)	-44.90	-26.90	18.00	Fe8O8 (OH) 6SO4
Sepiolite	-5.39	10.45	15.84	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-8.21	10.45	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-0.82	-11.69	-10.87	FeCO3
SiO2 (a)	-1.14	-3.88	-2.74	SiO2
Sulfur	-4.04	0.91	4.95	S
Talc	-4.12	17.61	21.73	Mg3Si4O10 (OH) 2
Troilite	-0.23	-6.38	-6.15	FeS
Witherite	-4.91	-13.48	-8.57	BaCO3

End of simulation.

Reading input data for simulation 2.

SOLUTION 1 BB04W 9-6-2007
temp 22.2
pH 6.77
pe 4
redox S(-2)/S(6)
units mg/kgw

```

density  1
N        0.55
Fe       0.005
S(6)     1220 as SO4
S(-2)    0.42
Cl       804
Br       1.81
Alkalinity 1500 as HCO3
Ba       0.18
Ca       328
Mg       154
Na       960
K        17.8
Mn       0.02
Si       13.2
water    1 # kg

```

END

Beginning of initial solution calculations.

Initial solution 1. BB04W 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	2.458e-002	2.458e-002
Ba	1.311e-006	1.311e-006
Br	2.265e-005	2.265e-005
Ca	8.184e-003	8.184e-003
Cl	2.268e-002	2.268e-002
Fe	8.953e-008	8.953e-008
K	4.552e-004	4.552e-004
Mg	6.334e-003	6.334e-003
Mn	3.640e-007	3.640e-007
N	3.927e-005	3.927e-005
Na	4.176e-002	4.176e-002
S(-2)	1.310e-005	1.310e-005
S(6)	1.270e-002	1.270e-002
Si	2.197e-004	2.197e-004

-----Description of solution-----

```

pH = 6.770
pe = 4.000
Activity of water = 0.998
Ionic strength = 8.270e-002
Mass of water (kg) = 1.000e+000
Total carbon (mol/kg) = 3.170e-002
Total CO2 (mol/kg) = 3.170e-002
Temperature (deg C) = 22.200
Electrical balance (eq) = -1.411e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -1.11

```

Iterations = 11
 Total H = 1.110379e+002
 Total O = 5.564583e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2) / S (6)	-2.9959	-0.1756

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.036e-007	1.698e-007	-6.691	-6.770	-0.079
OH-	6.107e-008	4.745e-008	-7.214	-7.324	-0.110
H2O	5.551e+001	9.980e-001	1.744	-0.001	0.000
Ba	1.311e-006				
Ba+2	7.349e-007	2.951e-007	-6.134	-6.530	-0.396
BaSO4	5.149e-007	5.248e-007	-6.288	-6.280	0.008
BaHCO3+	6.008e-008	4.765e-008	-7.221	-7.322	-0.101
BaCO3	6.775e-010	6.905e-010	-9.169	-9.161	0.008
BaOH+	7.408e-014	5.876e-014	-13.130	-13.231	-0.101
Br	2.265e-005				
Br-	2.265e-005	1.744e-005	-4.645	-4.759	-0.114
C (4)	3.170e-002				
HCO3-	2.298e-002	1.840e-002	-1.639	-1.735	-0.097
CO2	7.165e-003	7.303e-003	-2.145	-2.136	0.008
CaHCO3+	6.789e-004	5.435e-004	-3.168	-3.265	-0.097
MgHCO3+	5.055e-004	4.009e-004	-3.296	-3.397	-0.101
NaHCO3	3.285e-004	3.349e-004	-3.483	-3.475	0.008
CaCO3	1.814e-005	1.849e-005	-4.741	-4.733	0.008
CO3-2	1.166e-005	4.792e-006	-4.933	-5.320	-0.386
MgCO3	8.097e-006	8.252e-006	-5.092	-5.083	0.008
NaCO3-	3.157e-006	2.504e-006	-5.501	-5.601	-0.101
MnHCO3+	1.374e-007	1.090e-007	-6.862	-6.963	-0.101
BaHCO3+	6.008e-008	4.765e-008	-7.221	-7.322	-0.101
FeHCO3+	3.709e-008	2.942e-008	-7.431	-7.531	-0.101
MnCO3	2.483e-008	2.530e-008	-7.605	-7.597	0.008
FeCO3	1.803e-009	1.838e-009	-8.744	-8.736	0.008
BaCO3	6.775e-010	6.905e-010	-9.169	-9.161	0.008
Fe (CO3) (OH) -	5.298e-011	4.202e-011	-10.276	-10.377	-0.101
Fe (CO3) 2-2	2.614e-011	1.035e-011	-10.583	-10.985	-0.403
Ca	8.184e-003				
Ca+2	5.847e-003	2.423e-003	-2.233	-2.616	-0.383
CaSO4	1.639e-003	1.671e-003	-2.785	-2.777	0.008
CaHCO3+	6.789e-004	5.435e-004	-3.168	-3.265	-0.097
CaCO3	1.814e-005	1.849e-005	-4.741	-4.733	0.008
CaOH+	2.979e-009	2.363e-009	-8.526	-8.627	-0.101
CaHSO4+	2.026e-009	1.607e-009	-8.693	-8.794	-0.101
Cl	2.268e-002				
Cl-	2.268e-002	1.767e-002	-1.644	-1.753	-0.108
MnCl+	6.033e-009	4.785e-009	-8.219	-8.320	-0.101

FeCl+	4.917e-010	3.900e-010	-9.308	-9.409	-0.101
MnCl2	3.621e-011	3.691e-011	-10.441	-10.433	0.008
MnCl3-	2.265e-013	1.796e-013	-12.645	-12.746	-0.101
FeCl+2	1.628e-024	6.442e-025	-23.788	-24.191	-0.403
FeCl2+	7.011e-026	5.561e-026	-25.154	-25.255	-0.101
FeCl3	9.641e-029	9.826e-029	-28.016	-28.008	0.008
Fe (2)	8.953e-008				
Fe+2	3.769e-008	1.599e-008	-7.424	-7.796	-0.372
FeHCO3+	3.709e-008	2.942e-008	-7.431	-7.531	-0.101
FeSO4	9.401e-009	9.582e-009	-8.027	-8.019	0.008
FeS	2.655e-009	2.706e-009	-8.576	-8.568	0.008
FeCO3	1.803e-009	1.838e-009	-8.744	-8.736	0.008
FeCl+	4.917e-010	3.900e-010	-9.308	-9.409	-0.101
Fe (HS) 2	2.901e-010	2.956e-010	-9.538	-9.529	0.008
Fe (CO3) (OH) -	5.298e-011	4.202e-011	-10.276	-10.377	-0.101
FeOH+	3.033e-011	2.406e-011	-10.518	-10.619	-0.101
Fe (CO3) 2-2	2.614e-011	1.035e-011	-10.583	-10.985	-0.403
Fe (HS) 3-	1.849e-013	1.466e-013	-12.733	-12.834	-0.101
FeHSO4+	1.337e-014	1.060e-014	-13.874	-13.975	-0.101
Fe (OH) 2	1.330e-015	1.355e-015	-14.876	-14.868	0.008
Fe (3)	1.426e-016				
Fe (OH) 2+	9.349e-017	7.415e-017	-16.029	-16.130	-0.101
Fe (OH) 3	4.869e-017	4.963e-017	-16.313	-16.304	0.008
Fe (OH) 4-	2.993e-019	2.374e-019	-18.524	-18.624	-0.101
FeOH+2	1.072e-019	4.242e-020	-18.970	-19.372	-0.403
FeSO4+	6.085e-023	4.826e-023	-22.216	-22.316	-0.101
Fe+3	6.767e-024	1.320e-024	-23.170	-23.879	-0.710
Fe (SO4) 2-	4.672e-024	3.706e-024	-23.330	-23.431	-0.101
FeCl+2	1.628e-024	6.442e-025	-23.788	-24.191	-0.403
FeCl2+	7.011e-026	5.561e-026	-25.154	-25.255	-0.101
FeCl3	9.641e-029	9.826e-029	-28.016	-28.008	0.008
FeHSO4+2	5.558e-029	2.199e-029	-28.255	-28.658	-0.403
Fe2 (OH) 2+4	2.219e-036	5.442e-038	-35.654	-37.264	-1.610
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-48.445	-50.961	-2.516
H (0)	4.043e-011				
H2	2.022e-011	2.060e-011	-10.694	-10.686	0.008
K	4.552e-004				
K+	4.448e-004	3.466e-004	-3.352	-3.460	-0.108
KSO4-	1.037e-005	8.227e-006	-4.984	-5.085	-0.101
KOH	6.929e-012	7.063e-012	-11.159	-11.151	0.008
Mg	6.334e-003				
Mg+2	4.391e-003	1.884e-003	-2.357	-2.725	-0.367
MgSO4	1.430e-003	1.457e-003	-2.845	-2.836	0.008
MgHCO3+	5.055e-004	4.009e-004	-3.296	-3.397	-0.101
MgCO3	8.097e-006	8.252e-006	-5.092	-5.083	0.008
MgOH+	1.694e-008	1.344e-008	-7.771	-7.872	-0.101
Mn (2)	3.640e-007				
Mn+2	1.567e-007	6.648e-008	-6.805	-7.177	-0.372
MnHCO3+	1.374e-007	1.090e-007	-6.862	-6.963	-0.101
MnSO4	3.900e-008	3.975e-008	-7.409	-7.401	0.008
MnCO3	2.483e-008	2.530e-008	-7.605	-7.597	0.008
MnCl+	6.033e-009	4.785e-009	-8.219	-8.320	-0.101
MnCl2	3.621e-011	3.691e-011	-10.441	-10.433	0.008
MnOH+	1.005e-011	7.975e-012	-10.998	-11.098	-0.101

MnCl3-	2.265e-013	1.796e-013	-12.645	-12.746	-0.101
Mn (NO3) 2	0.000e+000	0.000e+000	-169.559	-169.550	0.008
Mn (3)	1.105e-035				
Mn+3	1.105e-035	1.373e-036	-34.957	-35.862	-0.906
N (-3)	1.977e-005				
NH4+	1.890e-005	1.441e-005	-4.723	-4.841	-0.118
NH4SO4-	8.304e-007	6.586e-007	-6.081	-6.181	-0.101
NH3	3.884e-008	3.959e-008	-7.411	-7.402	0.008
N (0)	1.950e-005				
N2	9.748e-006	9.935e-006	-5.011	-5.003	0.008
N (3)	0.000e+000				
NO2-	0.000e+000	0.000e+000	-60.048	-60.161	-0.114
N (5)	0.000e+000				
NO3-	0.000e+000	0.000e+000	-81.374	-81.488	-0.114
Mn (NO3) 2	0.000e+000	0.000e+000	-169.559	-169.550	0.008
Na	4.176e-002				
Na+	4.071e-002	3.237e-002	-1.390	-1.490	-0.100
NaSO4-	7.129e-004	5.654e-004	-3.147	-3.248	-0.101
NaHCO3	3.285e-004	3.349e-004	-3.483	-3.475	0.008
NaCO3-	3.157e-006	2.504e-006	-5.501	-5.601	-0.101
NaOH	1.233e-009	1.257e-009	-8.909	-8.901	0.008
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-71.930	-71.922	0.008
S (-2)	1.310e-005				
H2S	7.233e-006	7.372e-006	-5.141	-5.132	0.008
HS-	5.862e-006	4.555e-006	-5.232	-5.342	-0.110
FeS	2.655e-009	2.706e-009	-8.576	-8.568	0.008
Fe (HS) 2	2.901e-010	2.956e-010	-9.538	-9.529	0.008
S-2	6.648e-012	2.669e-012	-11.177	-11.574	-0.396
Fe (HS) 3-	1.849e-013	1.466e-013	-12.733	-12.834	-0.101
S (6)	1.270e-002				
SO4-2	8.906e-003	3.549e-003	-2.050	-2.450	-0.400
CaSO4	1.639e-003	1.671e-003	-2.785	-2.777	0.008
MgSO4	1.430e-003	1.457e-003	-2.845	-2.836	0.008
NaSO4-	7.129e-004	5.654e-004	-3.147	-3.248	-0.101
KSO4-	1.037e-005	8.227e-006	-4.984	-5.085	-0.101
NH4SO4-	8.304e-007	6.586e-007	-6.081	-6.181	-0.101
BaSO4	5.149e-007	5.248e-007	-6.288	-6.280	0.008
HSO4-	6.955e-008	5.516e-008	-7.158	-7.258	-0.101
MnSO4	3.900e-008	3.975e-008	-7.409	-7.401	0.008
FeSO4	9.401e-009	9.582e-009	-8.027	-8.019	0.008
CaHSO4+	2.026e-009	1.607e-009	-8.693	-8.794	-0.101
FeHSO4+	1.337e-014	1.060e-014	-13.874	-13.975	-0.101
FeSO4+	6.085e-023	4.826e-023	-22.216	-22.316	-0.101
Fe (SO4) 2-	4.672e-024	3.706e-024	-23.330	-23.431	-0.101
FeHSO4+2	5.558e-029	2.199e-029	-28.255	-28.658	-0.403
Si	2.197e-004				
H4SiO4	2.195e-004	2.237e-004	-3.659	-3.650	0.008
H3SiO4-	2.217e-007	1.759e-007	-6.654	-6.755	-0.101
H2SiO4-2	1.479e-013	5.853e-014	-12.830	-13.233	-0.403

-----Saturation indices-----

Phase

SI log IAP log KT

[Fe2(OH)5]	-7.83	15.26	23.09	Fe2(OH)5
[Fe3(OH)7]	-3.99	21.00	24.99	Fe3(OH)7
[Fe3(OH)8]	-17.35	24.77	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-35.21	23.14	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-34.37	26.01	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-25.34	18.22	43.56	Fe4(OH)8(Cl)1
Anhydrite	-0.72	-5.07	-4.35	CaSO4
Aragonite	0.38	-7.94	-8.32	CaCO3
Barite	1.04	-8.98	-10.02	BaSO4
Brucite	-5.98	10.81	16.79	Mg(OH)2
Calcite	0.53	-7.94	-8.46	CaCO3
Chalcedony	-0.06	-3.65	-3.58	SiO2
Chrysotile	-7.41	25.14	32.55	Mg3Si2O5(OH)4
CO2(g)	-0.70	-2.14	-1.43	CO2
Dolomite	1.04	-15.98	-17.02	CaMg(CO3)2
Epsomite	-3.02	-5.18	-2.16	MgSO4·7H2O
Fe(OH)2(1)	-7.20	5.74	12.94	Fe(OH)2
Fe(OH)2(2)	-8.15	5.74	13.89	Fe(OH)2
Fe(OH)3(a)	-8.46	-3.57	4.89	Fe(OH)3
FeO	-7.85	5.74	13.59	FeO
FeS(am)	-2.49	-6.37	-3.88	FeS
FeS(ppt)	-2.45	-6.37	-3.92	FeS
Goethite	-2.67	-3.57	-0.90	FeOOH
Greigite	-11.13	-49.84	-38.71	Fe3S4
Gypsum	-0.49	-5.07	-4.58	CaSO4·2H2O
H2(g)	-7.55	-10.69	-3.14	H2
H2O(g)	-1.58	-0.00	1.58	H2O
H2S(g)	-4.17	-5.13	-0.97	H2S
Halite	-4.82	-3.24	1.58	NaCl
Hausmannite	-35.10	26.63	61.73	Mn3O4
Hematite	-3.35	-7.14	-3.79	Fe2O3
Jarosite-H3O	-30.97	-42.69	-11.73	H3OFe3(SO4)2(OH)6
Jarosite-K	-28.46	-39.38	-10.93	KFe3(SO4)2(OH)6
Lepidocrocite	-7.18	9.52	16.70	FeOOH
Lime	-11.89	10.92	22.81	Ca(OH)2
Mackinawite	-1.75	-6.37	-4.62	FeS
Mackinawite(2)	-2.89	0.61	3.50	FeS
Magnetite	-21.02	24.78	45.80	Fe3O4
Manganite	-15.20	10.14	25.34	MnOOH
Marcasite	6.90	-10.93	-17.84	FeS2
Melanterite	-8.01	-10.25	-2.24	FeSO4·7H2O
N2(g)	-1.75	-5.00	-3.25	N2
Nesquehonite	-2.47	-8.05	-5.58	MgCO3·3H2O
NH3(g)	-9.23	-7.40	1.83	NH3
O2(g)	-68.97	-71.92	-2.95	O2
Pyrite	7.63	-10.93	-18.56	FeS2
Pyrochroite	-8.84	6.36	15.20	Mn(OH)2
Pyrolusite	-27.92	13.91	41.83	MnO2
Quartz	0.37	-3.65	-4.02	SiO2
Rhodochrosite	-1.38	-12.50	-11.12	MnCO3
Schwertmannite(1)	-67.85	-57.35	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-62.56	-44.56	18.00	Fe8O8(OH)6SO4
Sepiolite	-5.15	10.68	15.83	Mg2Si3O7.5OH:3H2O

Sepiolite(d)	-7.98	10.68	18.66	Mg ₂ Si ₃ O ₇ .5OH:3H ₂ O
Siderite	-2.24	-13.12	-10.87	FeCO ₃
SiO ₂ (a)	-0.91	-3.65	-2.74	SiO ₂
Sulfur	-2.53	2.42	4.95	S
Talc	-3.87	17.85	21.72	Mg ₃ Si ₄ O ₁₀ (OH) ₂
Troilite	-0.21	-6.37	-6.15	FeS
Witherite	-3.28	-11.85	-8.57	BaCO ₃

End of simulation.

Reading input data for simulation 3.

SOLUTION 1 BB04D 9-6-2007

temp	22.5
pH	6.71
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
N	0.152
Fe	0.25
S(6)	1690 as SO ₄
S(-2)	0.005
Cl	770
Br	3.83
Alkalinity	950 as HCO ₃
Ba	0.01
Ca	365
Mg	168
Na	893
K	8.88
Mn	0.65
Si	9.05
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. BB04D 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.557e-002	1.557e-002
Ba	7.281e-008	7.281e-008
Br	4.793e-005	4.793e-005
Ca	9.107e-003	9.107e-003
Cl	2.172e-002	2.172e-002

Fe	4.477e-006	4.477e-006
K	2.271e-004	2.271e-004
Mg	6.910e-003	6.910e-003
Mn	1.183e-005	1.183e-005
N	1.085e-005	1.085e-005
Na	3.884e-002	3.884e-002
S (-2)	1.559e-007	1.559e-007
S (6)	1.759e-002	1.759e-002
Si	1.506e-004	1.506e-004

-----Description of solution-----

pH	=	6.710
pe	=	4.000
Activity of water	=	0.998
Ionic strength	=	8.411e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	2.072e-002
Total CO2 (mol/kg)	=	2.072e-002
Temperature (deg C)	=	22.500
Electrical balance (eq)	=	-1.381e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	-1.13
Iterations	=	10
Total H	=	1.110286e+002
Total O	=	5.563417e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2)/S (6)	-2.6720	-0.1567

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.340e-007	1.950e-007	-6.631	-6.710	-0.079
OH-	5.455e-008	4.231e-008	-7.263	-7.374	-0.110
H2O	5.551e+001	9.981e-001	1.744	-0.001	0.000
Ba	7.281e-008				
Ba+2	3.631e-008	1.450e-008	-7.440	-7.839	-0.399
BaSO4	3.460e-008	3.528e-008	-7.461	-7.453	0.008
BaHCO3+	1.884e-009	1.493e-009	-8.725	-8.826	-0.101
BaCO3	1.854e-011	1.890e-011	-10.732	-10.724	0.008
BaOH+	3.175e-015	2.515e-015	-14.498	-14.600	-0.101
Br	4.793e-005				
Br-	4.793e-005	3.683e-005	-4.319	-4.434	-0.114
C (4)	2.072e-002				
HCO3-	1.454e-002	1.162e-002	-1.838	-1.935	-0.097
CO2	5.172e-003	5.274e-003	-2.286	-2.278	0.008
CaHCO3+	4.588e-004	3.668e-004	-3.338	-3.436	-0.097
MgHCO3+	3.298e-004	2.612e-004	-3.482	-3.583	-0.101
NaHCO3	1.921e-004	1.958e-004	-3.717	-3.708	0.008

		CaCO ₃	1.073e-005	1.094e-005	-4.969	-4.961	0.008
		CO ₃ -2	6.494e-006	2.653e-006	-5.187	-5.576	-0.389
		MgCO ₃	4.639e-006	4.730e-006	-5.334	-5.325	0.008
		MnHCO ₃ +	3.238e-006	2.565e-006	-5.490	-5.591	-0.101
		NaCO ₃ -	1.646e-006	1.304e-006	-5.784	-5.885	-0.101
		FeHCO ₃ +	1.385e-006	1.097e-006	-5.859	-5.960	-0.101
		MnCO ₃	5.119e-007	5.219e-007	-6.291	-6.282	0.008
		FeCO ₃	5.893e-008	6.008e-008	-7.230	-7.221	0.008
		BaHCO ₃ +	1.884e-009	1.493e-009	-8.725	-8.826	-0.101
		Fe (CO ₃) (OH) -	1.511e-009	1.197e-009	-8.821	-8.922	-0.101
		Fe (CO ₃) 2-2	4.758e-010	1.873e-010	-9.323	-9.727	-0.405
		BaCO ₃	1.854e-011	1.890e-011	-10.732	-10.724	0.008
Ca	9.107e-003						
		Ca+2	6.247e-003	2.575e-003	-2.204	-2.589	-0.385
		CaSO ₄	2.390e-003	2.437e-003	-2.622	-2.613	0.008
		CaHCO ₃ +	4.588e-004	3.668e-004	-3.338	-3.436	-0.097
		CaCO ₃	1.073e-005	1.094e-005	-4.969	-4.961	0.008
		CaHSO ₄ +	3.409e-009	2.700e-009	-8.467	-8.569	-0.101
		CaOH+	2.762e-009	2.188e-009	-8.559	-8.660	-0.101
Cl	2.172e-002						
		Cl-	2.172e-002	1.689e-002	-1.663	-1.772	-0.109
		MnCl+	2.151e-007	1.704e-007	-6.667	-6.768	-0.101
		FeCl+	2.779e-008	2.201e-008	-7.556	-7.657	-0.101
		MnCl ₂	1.233e-009	1.257e-009	-8.909	-8.901	0.008
		MnCl ₃ -	7.383e-012	5.848e-012	-11.132	-11.233	-0.101
		FeCl+2	1.999e-022	7.870e-023	-21.699	-22.104	-0.405
		FeCl ₂ +	8.122e-024	6.433e-024	-23.090	-23.192	-0.101
		FeCl ₃	1.066e-026	1.087e-026	-25.972	-25.964	0.008
Fe (2)	4.477e-006						
		Fe+2	2.236e-006	9.439e-007	-5.650	-6.025	-0.375
		FeHCO ₃ +	1.385e-006	1.097e-006	-5.859	-5.960	-0.101
		FeSO ₄	7.634e-007	7.783e-007	-6.117	-6.109	0.008
		FeCO ₃	5.893e-008	6.008e-008	-7.230	-7.221	0.008
		FeCl+	2.779e-008	2.201e-008	-7.556	-7.657	-0.101
		FeOH+	1.598e-009	1.266e-009	-8.796	-8.898	-0.101
		Fe (CO ₃) (OH) -	1.511e-009	1.197e-009	-8.821	-8.922	-0.101
		FeS	1.495e-009	1.524e-009	-8.825	-8.817	0.008
		Fe (CO ₃) 2-2	4.758e-010	1.873e-010	-9.323	-9.727	-0.405
		Fe (HS) 2	2.055e-012	2.095e-012	-11.687	-11.679	0.008
		FeHSO ₄ +	1.249e-012	9.897e-013	-11.903	-12.005	-0.101
		Fe (OH) 2	5.956e-014	6.072e-014	-13.225	-13.217	0.008
		Fe (HS) 3-	1.437e-017	1.138e-017	-16.842	-16.944	-0.101
Fe (3)	1.354e-014						
		Fe (OH) 2+	9.259e-015	7.334e-015	-14.033	-14.135	-0.101
		Fe (OH) 3	4.250e-015	4.333e-015	-14.372	-14.363	0.008
		Fe (OH) 4-	2.308e-017	1.828e-017	-16.637	-16.738	-0.101
		FeOH+2	1.209e-017	4.761e-018	-16.917	-17.322	-0.405
		FeSO ₄ +	1.062e-020	8.413e-021	-19.974	-20.075	-0.101
		Fe (SO ₄) 2-	1.117e-021	8.849e-022	-20.952	-21.053	-0.101
		Fe+3	8.635e-022	1.671e-022	-21.064	-21.777	-0.713
		FeCl+2	1.999e-022	7.870e-023	-21.699	-22.104	-0.405
		FeCl ₂ +	8.122e-024	6.433e-024	-23.090	-23.192	-0.101
		FeHSO ₄ +2	1.118e-026	4.401e-027	-25.952	-26.356	-0.405
		FeCl ₃	1.066e-026	1.087e-026	-25.972	-25.964	0.008

Fe2 (OH) 2+4	2.820e-032	6.771e-034	-31.550	-33.169	-1.620
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-42.352	-44.883	-2.531
H (0)	1.195e-011				
H2	5.977e-012	6.094e-012	-11.224	-11.215	0.008
K	2.271e-004				
K+	2.200e-004	1.712e-004	-3.657	-3.767	-0.109
KSO4-	7.055e-006	5.588e-006	-5.152	-5.253	-0.101
KOH	2.980e-012	3.038e-012	-11.526	-11.517	0.008
Mg	6.910e-003				
Mg+2	4.545e-003	1.941e-003	-2.342	-2.712	-0.369
MgSO4	2.031e-003	2.070e-003	-2.692	-2.684	0.008
MgHCO3+	3.298e-004	2.612e-004	-3.482	-3.583	-0.101
MgCO3	4.639e-006	4.730e-006	-5.334	-5.325	0.008
MgOH+	1.565e-008	1.240e-008	-7.805	-7.907	-0.101
Mn (2)	1.183e-005				
Mn+2	5.867e-006	2.476e-006	-5.232	-5.606	-0.375
MnHCO3+	3.238e-006	2.565e-006	-5.490	-5.591	-0.101
MnSO4	1.998e-006	2.038e-006	-5.699	-5.691	0.008
MnCO3	5.119e-007	5.219e-007	-6.291	-6.282	0.008
MnCl+	2.151e-007	1.704e-007	-6.667	-6.768	-0.101
MnCl2	1.233e-009	1.257e-009	-8.909	-8.901	0.008
MnOH+	3.349e-010	2.653e-010	-9.475	-9.576	-0.101
MnCl3-	7.383e-012	5.848e-012	-11.132	-11.233	-0.101
Mn (NO3) 2	0.000e+000	0.000e+000	-165.594	-165.586	0.008
Mn (3)	9.181e-034				
Mn+3	9.181e-034	1.127e-034	-33.037	-33.948	-0.911
N (-3)	2.337e-006				
NH4+	2.201e-006	1.674e-006	-5.657	-5.776	-0.119
NH4SO4-	1.322e-007	1.047e-007	-6.879	-6.980	-0.101
NH3	4.016e-009	4.095e-009	-8.396	-8.388	0.008
N (0)	8.515e-006				
N2	4.257e-006	4.341e-006	-5.371	-5.362	0.008
N (3)	0.000e+000				
NO2-	0.000e+000	0.000e+000	-59.410	-59.525	-0.114
N (5)	0.000e+000				
NO3-	0.000e+000	0.000e+000	-80.176	-80.291	-0.114
Mn (NO3) 2	0.000e+000	0.000e+000	-165.594	-165.586	0.008
Na	3.884e-002				
Na+	3.774e-002	2.996e-002	-1.423	-1.523	-0.100
NaSO4-	9.059e-004	7.176e-004	-3.043	-3.144	-0.101
NaHCO3	1.921e-004	1.958e-004	-3.717	-3.708	0.008
NaCO3-	1.646e-006	1.304e-006	-5.784	-5.885	-0.101
NaOH	9.940e-010	1.013e-009	-9.003	-8.994	0.008
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-70.773	-70.765	0.008
S (-2)	1.559e-007				
H2S	9.010e-008	9.186e-008	-7.045	-7.037	0.008
HS-	6.434e-008	4.990e-008	-7.192	-7.302	-0.110
FeS	1.495e-009	1.524e-009	-8.825	-8.817	0.008
Fe (HS) 2	2.055e-012	2.095e-012	-11.687	-11.679	0.008
S-2	6.514e-014	2.601e-014	-13.186	-13.585	-0.399
Fe (HS) 3-	1.437e-017	1.138e-017	-16.842	-16.944	-0.101
S (6)	1.759e-002				
SO4-2	1.226e-002	4.855e-003	-1.912	-2.314	-0.402

CaSO4	2.390e-003	2.437e-003	-2.622	-2.613	0.008
MgSO4	2.031e-003	2.070e-003	-2.692	-2.684	0.008
NaSO4-	9.059e-004	7.176e-004	-3.043	-3.144	-0.101
KSO4-	7.055e-006	5.588e-006	-5.152	-5.253	-0.101
MnSO4	1.998e-006	2.038e-006	-5.699	-5.691	0.008
FeSO4	7.634e-007	7.783e-007	-6.117	-6.109	0.008
NH4SO4-	1.322e-007	1.047e-007	-6.879	-6.980	-0.101
HSO4-	1.101e-007	8.721e-008	-6.958	-7.059	-0.101
BaSO4	3.460e-008	3.528e-008	-7.461	-7.453	0.008
CaHSO4+	3.409e-009	2.700e-009	-8.467	-8.569	-0.101
FeHSO4+	1.249e-012	9.897e-013	-11.903	-12.005	-0.101
FeSO4+	1.062e-020	8.413e-021	-19.974	-20.075	-0.101
Fe (SO4) 2-	1.117e-021	8.849e-022	-20.952	-21.053	-0.101
FeHSO4+2	1.118e-026	4.401e-027	-25.952	-26.356	-0.405
Si	1.506e-004				
H4SiO4	1.505e-004	1.534e-004	-3.822	-3.814	0.008
H3SiO4-	1.341e-007	1.062e-007	-6.873	-6.974	-0.101
H2SiO4-2	7.979e-014	3.141e-014	-13.098	-13.503	-0.405

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-4.27	18.82	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	1.23	26.22	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-11.87	30.25	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-24.91	33.44	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-23.68	36.70	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-18.43	25.13	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-0.55	-4.90	-4.35	CaSO4
Aragonite	0.16	-8.17	-8.32	CaCO3
Barite	-0.14	-10.15	-10.01	BaSO4
Brucite	-6.09	10.71	16.79	Mg (OH) 2
Calcite	0.30	-8.17	-8.47	CaCO3
Chalcedony	-0.23	-3.81	-3.58	SiO2
Chrysotile	-8.02	24.50	32.51	Mg3Si2O5 (OH) 4
CO2 (g)	-0.84	-2.28	-1.44	CO2
Dolomite	0.58	-16.45	-17.03	CaMg (CO3) 2
Epsomite	-2.87	-5.03	-2.16	MgSO4:7H2O
Fe (OH) 2 (1)	-5.55	7.39	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-6.50	7.39	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-6.54	-1.65	4.89	Fe (OH) 3
FeO	-6.20	7.39	13.59	FeO
FeS (am)	-2.73	-6.62	-3.88	FeS
FeS (ppt)	-2.70	-6.62	-3.92	FeS
Goethite	-0.74	-1.65	-0.91	FeOOH
Greigite	-13.23	-51.95	-38.71	Fe3S4
Gypsum	-0.32	-4.90	-4.58	CaSO4:2H2O
H2 (g)	-8.08	-11.22	-3.14	H2
H2O (g)	-1.58	-0.00	1.58	H2O
H2S (g)	-6.07	-7.04	-0.97	H2S
Halite	-4.87	-3.30	1.58	NaCl
Hausmannite	-30.14	31.51	61.65	Mn3O4
Hematite	0.52	-3.30	-3.82	Fe2O3

Jarosite-H3O	-24.65	-36.41	-11.77	H3OFe3 (SO4) 2 (OH) 6
Jarosite-K	-22.54	-33.47	-10.93	KFe3 (SO4) 2 (OH) 6
Lepidocrocite	-5.27	11.43	16.70	FeOOH
Lime	-11.98	10.83	22.81	Ca (OH) 2
Mackinawite	-2.00	-6.62	-4.62	FeS
Mackinawite(2)	-3.14	0.36	3.50	FeS
Magnetite	-15.54	30.26	45.80	Fe3O4
Manganite	-13.49	11.85	25.34	MnOOH
Marcasite	5.27	-12.55	-17.83	FeS2
Melanterite	-6.10	-8.34	-2.24	FeSO4:7H2O
N2(g)	-2.11	-5.36	-3.25	N2
Nesquehonite	-2.71	-8.29	-5.59	MgCO3:3H2O
NH3(g)	-10.21	-8.39	1.82	NH3
O2(g)	-67.82	-70.77	-2.95	O2
Pyrite	6.00	-12.55	-18.55	FeS2
Pyrochroite	-7.39	7.81	15.20	Mn (OH) 2
Pyrolusite	-25.90	15.89	41.78	MnO2
Quartz	0.21	-3.81	-4.02	SiO2
Rhodochrosite	-0.06	-11.18	-11.12	MnCO3
Schwertmannite(1)	-52.01	-41.51	10.50	Fe8O8 (OH) 4.4 (SO4) 1.8:8.4H2O
Schwertmannite(2)	-46.92	-28.92	18.00	Fe8O8 (OH) 6SO4
Sepiolite	-5.85	9.97	15.83	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-8.69	9.97	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-0.73	-11.60	-10.87	FeCO3
SiO2(a)	-1.08	-3.81	-2.73	SiO2
Sulfur	-3.90	1.04	4.94	S
Talc	-4.82	16.87	21.69	Mg3Si4O10 (OH) 2
Troilite	-0.46	-6.62	-6.15	FeS
Witherite	-4.85	-13.41	-8.57	BaCO3

End of simulation.

Reading input data for simulation 4.

SOLUTION 1 BB05U 9-6-2007

temp	22.6
pH	6.85
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
N	0.115
Fe	0.1
S(6)	1560 as SO4
S(-2)	0.03
Cl	419
Br	2.69
Alkalinity	650 as HCO3
Ba	0.01
Ca	227

Mg	161
Na	625
K	2.75
Mn	0.01
Si	11.1
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. BB05U 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.065e-002	1.065e-002
Ba	7.281e-008	7.281e-008
Br	3.367e-005	3.367e-005
Ca	5.664e-003	5.664e-003
Cl	1.182e-002	1.182e-002
Fe	1.791e-006	1.791e-006
K	7.033e-005	7.033e-005
Mg	6.622e-003	6.622e-003
Mn	1.820e-007	1.820e-007
N	8.210e-006	8.210e-006
Na	2.719e-002	2.719e-002
S(-2)	9.356e-007	9.356e-007
S(6)	1.624e-002	1.624e-002
Si	1.847e-004	1.847e-004

-----Description of solution-----

pH	=	6.850
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	6.447e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	1.329e-002
Total CO2 (mol/kg)	=	1.329e-002
Temperature (deg C)	=	22.600
Electrical balance (eq)	=	-3.148e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	-3.53
Iterations	=	10
Total H	=	1.110238e+002
Total O	=	5.560912e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.9366	-0.1723

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.673e-007	1.413e-007	-6.776	-6.850	-0.074
OH-	7.410e-008	5.889e-008	-7.130	-7.230	-0.100
H2O	5.551e+001	9.987e-001	1.744	-0.001	0.000
Ba	7.281e-008				
BaSO4	3.717e-008	3.772e-008	-7.430	-7.423	0.006
Ba+2	3.429e-008	1.484e-008	-7.465	-7.829	-0.364
BaHCO3+	1.342e-009	1.083e-009	-8.872	-8.965	-0.093
BaCO3	1.867e-011	1.895e-011	-10.729	-10.722	0.006
BaOH+	4.403e-015	3.555e-015	-14.356	-14.449	-0.093
Br	3.367e-005				
Br-	3.367e-005	2.655e-005	-4.473	-4.576	-0.103
C (4)	1.329e-002				
HCO3-	1.008e-002	8.215e-003	-1.997	-2.085	-0.089
CO2	2.656e-003	2.695e-003	-2.576	-2.569	0.006
MgHCO3+	2.288e-004	1.847e-004	-3.641	-3.733	-0.093
CaHCO3+	2.087e-004	1.701e-004	-3.680	-3.769	-0.089
NaHCO3	9.735e-005	9.881e-005	-4.012	-4.005	0.006
CaCO3	6.917e-006	7.021e-006	-5.160	-5.154	0.006
CO3-2	5.881e-006	2.594e-006	-5.231	-5.586	-0.355
MgCO3	4.564e-006	4.632e-006	-5.341	-5.334	0.006
NaCO3-	1.133e-006	9.147e-007	-5.946	-6.039	-0.093
FeHCO3+	4.367e-007	3.526e-007	-6.360	-6.453	-0.093
MnHCO3+	3.919e-008	3.164e-008	-7.407	-7.500	-0.093
FeCO3	2.632e-008	2.671e-008	-7.580	-7.573	0.006
MnCO3	8.775e-009	8.906e-009	-8.057	-8.050	0.006
BaHCO3+	1.342e-009	1.083e-009	-8.872	-8.965	-0.093
Fe (CO3) (OH) -	9.101e-010	7.348e-010	-9.041	-9.134	-0.093
Fe (CO3) 2-2	1.916e-010	8.143e-011	-9.718	-10.089	-0.372
BaCO3	1.867e-011	1.895e-011	-10.729	-10.722	0.006
Ca	5.664e-003				
Ca+2	3.804e-003	1.687e-003	-2.420	-2.773	-0.353
CaSO4	1.645e-003	1.669e-003	-2.784	-2.778	0.006
CaHCO3+	2.087e-004	1.701e-004	-3.680	-3.769	-0.089
CaCO3	6.917e-006	7.021e-006	-5.160	-5.154	0.006
CaOH+	2.451e-009	1.979e-009	-8.611	-8.703	-0.093
CaHSO4+	1.661e-009	1.341e-009	-8.780	-8.872	-0.093
Cl	1.182e-002				
Cl-	1.182e-002	9.414e-003	-1.927	-2.026	-0.099
FeCl+	6.908e-009	5.578e-009	-8.161	-8.254	-0.093
MnCl+	2.053e-009	1.657e-009	-8.688	-8.781	-0.093
MnCl2	6.711e-012	6.811e-012	-11.173	-11.167	0.006
MnCl3-	2.187e-014	1.766e-014	-13.660	-13.753	-0.093
FeCl+2	2.574e-023	1.094e-023	-22.589	-22.961	-0.372
FeCl2+	6.151e-025	4.967e-025	-24.211	-24.304	-0.093
FeCl3	4.607e-028	4.676e-028	-27.337	-27.330	0.006
Fe (2)	1.791e-006				
Fe+2	9.468e-007	4.292e-007	-6.024	-6.367	-0.344
FeHCO3+	4.367e-007	3.526e-007	-6.360	-6.453	-0.093
FeSO4	3.650e-007	3.704e-007	-6.438	-6.431	0.006

FeCO ₃	2.632e-008	2.671e-008	-7.580	-7.573	0.006
FeCl ⁺	6.908e-009	5.578e-009	-8.161	-8.254	-0.093
FeS	6.831e-009	6.934e-009	-8.165	-8.159	0.006
FeOH ⁺	9.920e-010	8.009e-010	-9.003	-9.096	-0.093
Fe (CO ₃) (OH) -	9.101e-010	7.348e-010	-9.041	-9.134	-0.093
Fe (CO ₃) 2-2	1.916e-010	8.143e-011	-9.718	-10.089	-0.372
Fe (HS) 2	4.929e-011	5.003e-011	-10.307	-10.301	0.006
FeHSO ₄ ⁺	4.227e-013	3.413e-013	-12.374	-12.467	-0.093
Fe (OH) 2	5.189e-014	5.267e-014	-13.285	-13.278	0.006
Fe (HS) 3-	2.440e-015	1.970e-015	-14.613	-14.705	-0.093
Fe (3)	7.212e-015				
Fe (OH) 2 ⁺	4.350e-015	3.513e-015	-14.361	-14.454	-0.093
Fe (OH) 3	2.837e-015	2.879e-015	-14.547	-14.541	0.006
Fe (OH) 4-	2.086e-017	1.684e-017	-16.681	-16.774	-0.093
FeOH+2	3.870e-018	1.645e-018	-17.412	-17.784	-0.372
FeSO ₄ ⁺	2.712e-021	2.190e-021	-20.567	-20.660	-0.093
Fe (SO ₄) 2-	2.982e-022	2.407e-022	-21.526	-21.618	-0.093
Fe+3	1.910e-022	4.154e-023	-21.719	-22.382	-0.663
FeCl+2	2.574e-023	1.094e-023	-22.589	-22.961	-0.372
FeCl ₂ ⁺	6.151e-025	4.967e-025	-24.211	-24.304	-0.093
FeHSO ₄ +2	1.952e-027	8.298e-028	-26.709	-27.081	-0.372
FeCl ₃	4.607e-028	4.676e-028	-27.337	-27.330	0.006
Fe ₂ (OH) 2+4	2.466e-033	8.045e-035	-32.608	-34.094	-1.487
Fe ₃ (OH) 4+5	0.000e+000	0.000e+000	-43.809	-46.132	-2.323
H (0)	2.130e-011				
H ₂	1.065e-011	1.081e-011	-10.973	-10.966	0.006
K	7.033e-005				
K ⁺	6.804e-005	5.420e-005	-4.167	-4.266	-0.099
KSO ₄ -	2.294e-006	1.852e-006	-5.639	-5.732	-0.093
KOH	1.309e-012	1.329e-012	-11.883	-11.877	0.006
Mg	6.622e-003				
Mg+2	4.252e-003	1.941e-003	-2.371	-2.712	-0.340
MgSO ₄	2.137e-003	2.169e-003	-2.670	-2.664	0.006
MgHCO ₃ ⁺	2.288e-004	1.847e-004	-3.641	-3.733	-0.093
MgCO ₃	4.564e-006	4.632e-006	-5.341	-5.334	0.006
MgOH ⁺	2.141e-008	1.728e-008	-7.669	-7.762	-0.093
Mn (2)	1.820e-007				
Mn+2	9.532e-008	4.321e-008	-7.021	-7.364	-0.344
MnHCO ₃ ⁺	3.919e-008	3.164e-008	-7.407	-7.500	-0.093
MnSO ₄	3.667e-008	3.722e-008	-7.436	-7.429	0.006
MnCO ₃	8.775e-009	8.906e-009	-8.057	-8.050	0.006
MnCl ⁺	2.053e-009	1.657e-009	-8.688	-8.781	-0.093
MnOH ⁺	7.986e-012	6.448e-012	-11.098	-11.191	-0.093
MnCl ₂	6.711e-012	6.811e-012	-11.173	-11.167	0.006
MnCl ₃ -	2.187e-014	1.766e-014	-13.660	-13.753	-0.093
Mn (NO ₃) 2	0.000e+000	0.000e+000	-168.452	-168.446	0.006
Mn (3)	7.442e-036				
Mn+3	7.442e-036	1.085e-036	-35.128	-35.964	-0.836
N (-3)	2.998e-006				
NH ₄ ⁺	2.812e-006	2.200e-006	-5.551	-5.658	-0.107
NH ₄ SO ₄ -	1.781e-007	1.438e-007	-6.749	-6.842	-0.093
NH ₃	7.372e-009	7.482e-009	-8.132	-8.126	0.006
N (0)	5.212e-006				
N ₂	2.606e-006	2.645e-006	-5.584	-5.578	0.006

N (3)	0.000e+000					
NO2-	0.000e+000	0.000e+000	-59.735	-59.838	-0.103	
N (5)	0.000e+000					
NO3-	0.000e+000	0.000e+000	-80.739	-80.842	-0.103	
Mn (NO3) 2	0.000e+000	0.000e+000	-168.452	-168.446	0.006	
Na	2.719e-002					
Na+	2.642e-002	2.139e-002	-1.578	-1.670	-0.092	
NaSO4-	6.633e-004	5.355e-004	-3.178	-3.271	-0.093	
NaHCO3	9.735e-005	9.881e-005	-4.012	-4.005	0.006	
NaCO3-	1.133e-006	9.147e-007	-5.946	-6.039	-0.093	
NaOH	9.845e-010	9.992e-010	-9.007	-9.000	0.006	
O (0)	0.000e+000					
O2	0.000e+000	0.000e+000	-71.236	-71.229	0.006	
S (-2)	9.356e-007					
H2S	4.737e-007	4.808e-007	-6.325	-6.318	0.006	
HS-	4.550e-007	3.616e-007	-6.342	-6.442	-0.100	
FeS	6.831e-009	6.934e-009	-8.165	-8.159	0.006	
Fe (HS) 2	4.929e-011	5.003e-011	-10.307	-10.301	0.006	
S-2	6.054e-013	2.620e-013	-12.218	-12.582	-0.364	
Fe (HS) 3-	2.440e-015	1.970e-015	-14.613	-14.705	-0.093	
S (6)	1.624e-002					
SO4-2	1.179e-002	5.073e-003	-1.928	-2.295	-0.366	
MgSO4	2.137e-003	2.169e-003	-2.670	-2.664	0.006	
CaSO4	1.645e-003	1.669e-003	-2.784	-2.778	0.006	
NaSO4-	6.633e-004	5.355e-004	-3.178	-3.271	-0.093	
KSO4-	2.294e-006	1.852e-006	-5.639	-5.732	-0.093	
FeSO4	3.650e-007	3.704e-007	-6.438	-6.431	0.006	
NH4SO4-	1.781e-007	1.438e-007	-6.749	-6.842	-0.093	
HSO4-	8.192e-008	6.614e-008	-7.087	-7.180	-0.093	
BaSO4	3.717e-008	3.772e-008	-7.430	-7.423	0.006	
MnSO4	3.667e-008	3.722e-008	-7.436	-7.429	0.006	
CaHSO4+	1.661e-009	1.341e-009	-8.780	-8.872	-0.093	
FeHSO4+	4.227e-013	3.413e-013	-12.374	-12.467	-0.093	
FeSO4+	2.712e-021	2.190e-021	-20.567	-20.660	-0.093	
Fe (SO4) 2-	2.982e-022	2.407e-022	-21.526	-21.618	-0.093	
FeHSO4+2	1.952e-027	8.298e-028	-26.709	-27.081	-0.372	
Si	1.847e-004					
H4SiO4	1.845e-004	1.873e-004	-3.734	-3.728	0.006	
H3SiO4-	2.224e-007	1.796e-007	-6.653	-6.746	-0.093	
H2SiO4-2	1.737e-013	7.381e-014	-12.760	-13.132	-0.372	

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-4.51	18.58	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	0.92	25.91	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-12.30	29.82	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-25.82	32.53	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-24.56	35.82	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-19.20	24.36	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-0.72	-5.07	-4.35	CaSO4
Aragonite	-0.04	-8.36	-8.32	CaCO3
Barite	-0.11	-10.12	-10.01	BaSO4

Brucite	-5.81	10.99	16.79	Mg (OH) 2
Calcite	0.11	-8.36	-8.47	CaCO3
Chalcedony	-0.15	-3.73	-3.58	SiO2
Chrysotile	-6.99	25.51	32.50	Mg3Si2O5 (OH) 4
CO2 (g)	-1.13	-2.57	-1.44	CO2
Dolomite	0.38	-16.66	-17.03	CaMg (CO3) 2
Epsomite	-2.85	-5.01	-2.16	MgSO4:7H2O
Fe (OH) 2 (1)	-5.61	7.33	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-6.56	7.33	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-6.72	-1.83	4.89	Fe (OH) 3
FeO	-6.26	7.33	13.59	FeO
FeS (am)	-2.07	-5.96	-3.88	FeS
FeS (ppt)	-2.04	-5.96	-3.92	FeS
Goethite	-0.92	-1.83	-0.91	FeOOH
Greigite	-10.78	-49.50	-38.72	Fe3S4
Gypsum	-0.49	-5.07	-4.58	CaSO4:2H2O
H2 (g)	-7.83	-10.97	-3.14	H2
H2O (g)	-1.57	-0.00	1.57	H2O
H2S (g)	-5.35	-6.32	-0.97	H2S
Halite	-5.27	-3.70	1.58	NaCl
Hausmannite	-34.80	26.83	61.63	Mn3O4
Hematite	0.16	-3.66	-3.82	Fe2O3
Jarosite-H3O	-25.71	-37.49	-11.78	H3OFe3 (SO4) 2 (OH) 6
Jarosite-K	-23.97	-34.90	-10.94	KFe3 (SO4) 2 (OH) 6
Lepidocrocite	-5.46	11.24	16.70	FeOOH
Lime	-11.88	10.93	22.81	Ca (OH) 2
Mackinawite	-1.34	-5.96	-4.62	FeS
Mackinawite(2)	-2.49	1.01	3.50	FeS
Magnetite	-15.98	29.82	45.80	Fe3O4
Manganite	-15.09	10.25	25.34	MnOOH
Marcasite	6.40	-11.42	-17.83	FeS2
Melanterite	-6.43	-8.67	-2.24	FeSO4:7H2O
N2 (g)	-2.33	-5.58	-3.25	N2
Nesquehonite	-2.71	-8.30	-5.59	MgCO3:3H2O
NH3 (g)	-9.94	-8.13	1.82	NH3
O2 (g)	-68.28	-71.23	-2.95	O2
Pyrite	7.12	-11.42	-18.55	FeS2
Pyrochroite	-8.87	6.33	15.20	Mn (OH) 2
Pyrolusite	-27.61	14.16	41.77	MnO2
Quartz	0.29	-3.73	-4.02	SiO2
Rhodochrosite	-1.83	-12.95	-11.12	MnCO3
Schwertmannite(1)	-53.95	-43.45	10.50	Fe8O8 (OH) 4.4 (SO4) 1.8:8.4H2O
Schwertmannite(2)	-48.65	-30.65	18.00	Fe8O8 (OH) 6SO4
Sepiolite	-5.03	10.79	15.82	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-7.87	10.79	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-1.08	-11.95	-10.88	FeCO3
SiO2 (a)	-0.99	-3.73	-2.73	SiO2
Sulfur	-3.43	1.51	4.94	S
Talc	-3.62	18.06	21.67	Mg3Si4O10 (OH) 2
Troilite	0.20	-5.96	-6.15	FeS
Witherite	-4.85	-13.41	-8.57	BaCO3

End of simulation.

Reading input data for simulation 5.

SOLUTION 1 BB05W 9-6-2007

temp 21.2
pH 6.73
pe 4
redox S(-2)/S(6)
units mg/kgw
density 1
N 0.769
Fe 0.005
S(6) 1290 as SO4
S(-2) 0.35
Cl 839
Br 1.78
Alkalinity 1806 as HCO3
Ba 0.24
Ca 351
Mg 167
Na 1110
K 18.3
Mn 0.1
Si 14.8
water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. BB05W 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	2.960e-002	2.960e-002
Ba	1.747e-006	1.747e-006
Br	2.228e-005	2.228e-005
Ca	8.757e-003	8.757e-003
Cl	2.367e-002	2.367e-002
Fe	8.953e-008	8.953e-008
K	4.680e-004	4.680e-004
Mg	6.869e-003	6.869e-003
Mn	1.820e-006	1.820e-006
N	5.490e-005	5.490e-005
Na	4.828e-002	4.828e-002
S(-2)	1.092e-005	1.092e-005
S(6)	1.343e-002	1.343e-002
Si	2.463e-004	2.463e-004

-----Description of solution-----

pH = 6.730
 pe = 4.000
 Activity of water = 0.998
 Ionic strength = 9.118e-002
 Mass of water (kg) = 1.000e+000
 Total carbon (mol/kg) = 3.903e-002
 Total CO2 (mol/kg) = 3.903e-002
 Temperature (deg C) = 21.200
 Electrical balance (eq) = -1.063e-004
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.07
 Iterations = 11
 Total H = 1.110430e+002
 Total O = 5.566853e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.9169	-0.1704

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.243e-007	1.862e-007	-6.649	-6.730	-0.081
OH-	5.195e-008	4.000e-008	-7.284	-7.398	-0.114
H2O	5.551e+001	9.977e-001	1.744	-0.001	0.000
Ba	1.747e-006				
Ba+2	9.777e-007	3.813e-007	-6.010	-6.419	-0.409
BaSO4	6.786e-007	6.930e-007	-6.168	-6.159	0.009
BaHCO3+	9.029e-008	7.114e-008	-7.044	-7.148	-0.104
BaCO3	9.110e-010	9.304e-010	-9.040	-9.031	0.009
BaOH+	8.787e-014	6.923e-014	-13.056	-13.160	-0.104
Br	2.228e-005				
Br-	2.228e-005	1.698e-005	-4.652	-4.770	-0.118
C(4)	3.903e-002				
HCO3-	2.759e-002	2.194e-002	-1.559	-1.659	-0.100
CO2	9.486e-003	9.688e-003	-2.023	-2.014	0.009
CaHCO3+	8.274e-004	6.579e-004	-3.082	-3.182	-0.100
MgHCO3+	6.360e-004	5.011e-004	-3.197	-3.300	-0.104
NaHCO3	4.482e-004	4.577e-004	-3.349	-3.339	0.009
CaCO3	1.955e-005	1.997e-005	-4.709	-4.700	0.009
CO3-2	1.276e-005	5.097e-006	-4.894	-5.293	-0.398
MgCO3	8.908e-006	9.097e-006	-5.050	-5.041	0.009
NaCO3-	3.681e-006	2.900e-006	-5.434	-5.538	-0.104
MnHCO3+	7.555e-007	5.953e-007	-6.122	-6.225	-0.104
MnCO3	1.207e-007	1.233e-007	-6.918	-6.909	0.009
BaHCO3+	9.029e-008	7.114e-008	-7.044	-7.148	-0.104
FeHCO3+	4.101e-008	3.231e-008	-7.387	-7.491	-0.104
FeCO3	1.764e-009	1.801e-009	-8.754	-8.744	0.009
BaCO3	9.110e-010	9.304e-010	-9.040	-9.031	0.009

	Fe (CO3) (OH) -	4.766e-011	3.755e-011	-10.322	-10.425	-0.104
	Fe (CO3) 2-2	2.799e-011	1.079e-011	-10.553	-10.967	-0.414
Ca	8.757e-003					
	Ca+2	6.200e-003	2.503e-003	-2.208	-2.602	-0.394
	CaSO4	1.711e-003	1.747e-003	-2.767	-2.758	0.009
	CaHCO3+	8.274e-004	6.579e-004	-3.082	-3.182	-0.100
	CaCO3	1.955e-005	1.997e-005	-4.709	-4.700	0.009
	CaOH+	2.825e-009	2.226e-009	-8.549	-8.653	-0.104
	CaHSO4+	2.311e-009	1.821e-009	-8.636	-8.740	-0.104
Cl	2.367e-002					
	Cl-	2.367e-002	1.828e-002	-1.626	-1.738	-0.112
	MnCl+	2.878e-008	2.267e-008	-7.541	-7.644	-0.104
	FeCl+	4.718e-010	3.717e-010	-9.326	-9.430	-0.104
	MnCl2	1.772e-010	1.809e-010	-9.752	-9.743	0.009
	MnCl3-	1.156e-012	9.109e-013	-11.937	-12.041	-0.104
	FeCl+2	1.749e-024	6.741e-025	-23.757	-24.171	-0.414
	FeCl2+	7.893e-026	6.219e-026	-25.103	-25.206	-0.104
	FeCl3	1.113e-028	1.137e-028	-27.953	-27.944	0.009
Fe (2)	8.953e-008					
	FeHCO3+	4.101e-008	3.231e-008	-7.387	-7.491	-0.104
	Fe+2	3.563e-008	1.473e-008	-7.448	-7.832	-0.384
	FeSO4	8.669e-009	8.853e-009	-8.062	-8.053	0.009
	FeCO3	1.764e-009	1.801e-009	-8.754	-8.744	0.009
	FeS	1.725e-009	1.761e-009	-8.763	-8.754	0.009
	FeCl+	4.718e-010	3.717e-010	-9.326	-9.430	-0.104
	Fe (HS) 2	1.601e-010	1.635e-010	-9.796	-9.787	0.009
	Fe (CO3) (OH) -	4.766e-011	3.755e-011	-10.322	-10.425	-0.104
	Fe (CO3) 2-2	2.799e-011	1.079e-011	-10.553	-10.967	-0.414
	FeOH+	2.376e-011	1.872e-011	-10.624	-10.728	-0.104
	Fe (HS) 3-	7.972e-014	6.281e-014	-13.098	-13.202	-0.104
	FeHSO4+	1.360e-014	1.071e-014	-13.866	-13.970	-0.104
	Fe (OH) 2	1.017e-015	1.038e-015	-14.993	-14.984	0.009
Fe (3)	1.077e-016					
	Fe (OH) 2+	7.404e-017	5.834e-017	-16.131	-16.234	-0.104
	Fe (OH) 3	3.334e-017	3.405e-017	-16.477	-16.468	0.009
	Fe (OH) 4-	1.809e-019	1.425e-019	-18.743	-18.846	-0.104
	FeOH+2	9.873e-020	3.805e-020	-19.006	-19.420	-0.414
	FeSO4+	6.393e-023	5.037e-023	-22.194	-22.298	-0.104
	Fe+3	7.366e-024	1.380e-024	-23.133	-23.860	-0.727
	Fe (SO4) 2-	4.996e-024	3.936e-024	-23.301	-23.405	-0.104
	FeCl+2	1.749e-024	6.741e-025	-23.757	-24.171	-0.414
	FeCl2+	7.893e-026	6.219e-026	-25.103	-25.206	-0.104
	FeCl3	1.113e-028	1.137e-028	-27.953	-27.944	0.009
	FeHSO4+2	6.541e-029	2.521e-029	-28.184	-28.598	-0.414
	Fe2 (OH) 2+4	2.071e-036	4.568e-038	-35.684	-37.340	-1.656
	Fe3 (OH) 4+5	0.000e+000	0.000e+000	-48.512	-51.100	-2.588
H (0)	3.407e-011					
	H2	1.703e-011	1.739e-011	-10.769	-10.760	0.009
K	4.680e-004					
	K+	4.573e-004	3.533e-004	-3.340	-3.452	-0.112
	KSO4-	1.068e-005	8.415e-006	-4.971	-5.075	-0.104
	KOH	6.427e-012	6.563e-012	-11.192	-11.183	0.009
Mg	6.869e-003					
	Mg+2	4.730e-003	1.983e-003	-2.325	-2.703	-0.378

MgSO4	1.494e-003	1.526e-003	-2.826	-2.816	0.009
MgHCO3+	6.360e-004	5.011e-004	-3.197	-3.300	-0.104
MgCO3	8.908e-006	9.097e-006	-5.050	-5.041	0.009
MgOH+	1.492e-008	1.176e-008	-7.826	-7.930	-0.104
Mn (2)	1.820e-006				
MnHCO3+	7.555e-007	5.953e-007	-6.122	-6.225	-0.104
Mn+2	7.364e-007	3.045e-007	-6.133	-6.516	-0.384
MnSO4	1.786e-007	1.824e-007	-6.748	-6.739	0.009
MnCO3	1.207e-007	1.233e-007	-6.918	-6.909	0.009
MnCl+	2.878e-008	2.267e-008	-7.541	-7.644	-0.104
MnCl2	1.772e-010	1.809e-010	-9.752	-9.743	0.009
MnOH+	3.889e-011	3.064e-011	-10.410	-10.514	-0.104
MnCl3-	1.156e-012	9.109e-013	-11.937	-12.041	-0.104
Mn (NO3) 2	0.000e+000	0.000e+000	-169.185	-169.176	0.009
Mn (3)	5.550e-035				
Mn+3	5.550e-035	6.494e-036	-34.256	-35.187	-0.932
N (-3)	2.488e-005				
NH4+	2.378e-005	1.793e-005	-4.624	-4.746	-0.123
NH4SO4-	1.063e-006	8.377e-007	-5.973	-6.077	-0.104
NH3	4.094e-008	4.181e-008	-7.388	-7.379	0.009
N (0)	3.002e-005				
N2	1.501e-005	1.533e-005	-4.824	-4.814	0.009
N (3)	0.000e+000				
NO2-	0.000e+000	0.000e+000	-60.155	-60.273	-0.118
N (5)	0.000e+000				
NO3-	0.000e+000	0.000e+000	-81.514	-81.631	-0.118
Mn (NO3) 2	0.000e+000	0.000e+000	-169.185	-169.176	0.009
Na	4.828e-002				
Na+	4.700e-002	3.710e-002	-1.328	-1.431	-0.103
NaSO4-	8.351e-004	6.580e-004	-3.078	-3.182	-0.104
NaHCO3	4.482e-004	4.577e-004	-3.349	-3.339	0.009
NaCO3-	3.681e-006	2.900e-006	-5.434	-5.538	-0.104
NaOH	1.286e-009	1.313e-009	-8.891	-8.882	0.009
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-72.114	-72.105	0.009
S (-2)	1.092e-005				
H2S	6.331e-006	6.465e-006	-5.199	-5.189	0.009
HS-	4.583e-006	3.529e-006	-5.339	-5.452	-0.114
FeS	1.725e-009	1.761e-009	-8.763	-8.754	0.009
Fe (HS) 2	1.601e-010	1.635e-010	-9.796	-9.787	0.009
S-2	4.509e-012	1.758e-012	-11.346	-11.755	-0.409
Fe (HS) 3-	7.972e-014	6.281e-014	-13.098	-13.202	-0.104
S (6)	1.343e-002				
SO4-2	9.376e-003	3.626e-003	-2.028	-2.441	-0.413
CaSO4	1.711e-003	1.747e-003	-2.767	-2.758	0.009
MgSO4	1.494e-003	1.526e-003	-2.826	-2.816	0.009
NaSO4-	8.351e-004	6.580e-004	-3.078	-3.182	-0.104
KSO4-	1.068e-005	8.415e-006	-4.971	-5.075	-0.104
NH4SO4-	1.063e-006	8.377e-007	-5.973	-6.077	-0.104
BaSO4	6.786e-007	6.930e-007	-6.168	-6.159	0.009
MnSO4	1.786e-007	1.824e-007	-6.748	-6.739	0.009
HSO4-	7.679e-008	6.050e-008	-7.115	-7.218	-0.104
FeSO4	8.669e-009	8.853e-009	-8.062	-8.053	0.009
CaHSO4+	2.311e-009	1.821e-009	-8.636	-8.740	-0.104

FeHSO4+	1.360e-014	1.071e-014	-13.866	-13.970	-0.104
FeSO4+	6.393e-023	5.037e-023	-22.194	-22.298	-0.104
Fe (SO4) 2-	4.996e-024	3.936e-024	-23.301	-23.405	-0.104
FeHSO4+2	6.541e-029	2.521e-029	-28.184	-28.598	-0.414
Si	2.463e-004				
H4SiO4	2.461e-004	2.513e-004	-3.609	-3.600	0.009
H3SiO4-	2.206e-007	1.738e-007	-6.656	-6.760	-0.104
H2SiO4-2	1.279e-013	4.929e-014	-12.893	-13.307	-0.414

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH) 5]	-8.03	15.06	23.09	Fe2(OH) 5
[Fe3(OH) 7]	-4.30	20.69	24.99	Fe3(OH) 7
[Fe3(OH) 8]	-17.62	24.50	42.12	Fe3(OH) 8
[Fe6(OH) 12] [CO3]	-35.72	22.63	58.35	Fe6(OH) 12 (CO3) 1
[Fe6(OH) 12] [SO4]	-34.90	25.48	60.38	Fe6(OH) 12 (SO4) 1
[Fe6(OH) 8] [Cl]	-25.71	17.85	43.56	Fe4(OH) 8 (Cl) 1
Anhydrite	-0.69	-5.04	-4.35	CaSO4
Aragonite	0.42	-7.89	-8.31	CaCO3
Barite	1.17	-8.86	-10.03	BaSO4
Brucite	-6.04	10.76	16.79	Mg (OH) 2
Calcite	0.57	-7.89	-8.46	CaCO3
Chalcedony	-0.00	-3.60	-3.60	SiO2
Chrysotile	-7.61	25.07	32.68	Mg3Si2O5 (OH) 4
CO2 (g)	-0.59	-2.01	-1.42	CO2
Dolomite	1.11	-15.89	-17.00	CaMg (CO3) 2
Epsomite	-2.98	-5.15	-2.17	MgSO4:7H2O
Fe (OH) 2 (1)	-7.31	5.63	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-8.26	5.63	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-8.56	-3.67	4.89	Fe (OH) 3
FeO	-7.96	5.63	13.59	FeO
FeS (am)	-2.69	-6.55	-3.87	FeS
FeS (ppt)	-2.64	-6.55	-3.92	FeS
Goethite	-2.81	-3.67	-0.86	FeOOH
Greigite	-11.76	-50.44	-38.69	Fe3S4
Gypsum	-0.46	-5.04	-4.58	CaSO4:2H2O
H2 (g)	-7.63	-10.76	-3.13	H2
H2O (g)	-1.61	-0.00	1.61	H2O
H2S (g)	-4.24	-5.19	-0.95	H2S
Halite	-4.74	-3.17	1.57	NaCl
Hausmannite	-33.53	28.45	61.98	Mn3O4
Hematite	-3.63	-7.34	-3.72	Fe2O3
Jarosite-H3O	-31.23	-42.82	-11.59	H3OFe3 (SO4) 2 (OH) 6
Jarosite-K	-28.64	-39.54	-10.90	KFe3 (SO4) 2 (OH) 6
Lepidocrocite	-7.26	9.44	16.70	FeOOH
Lime	-11.95	10.86	22.81	Ca (OH) 2
Mackinawite	-1.95	-6.55	-4.61	FeS
Mackinawite (2)	-3.06	0.44	3.50	FeS
Magnetite	-21.29	24.51	45.80	Fe3O4
Manganite	-14.59	10.75	25.34	MnOOH
Marcasite	6.75	-11.11	-17.86	FeS2
Melanterite	-8.02	-10.28	-2.26	FeSO4:7H2O

N2(g)	-1.57	-4.81	-3.25	N2
Nesquehonite	-2.43	-8.00	-5.57	MgCO3:3H2O
NH3(g)	-9.23	-7.38	1.85	NH3
O2(g)	-69.16	-72.11	-2.94	O2
Pyrite	7.48	-11.11	-18.59	FeS2
Pyrochroite	-8.26	6.94	15.20	Mn(OH)2
Pyrolusite	-27.43	14.57	42.00	MnO2
Quartz	0.44	-3.60	-4.04	SiO2
Rhodochrosite	-0.69	-11.81	-11.12	MnCO3
Schwertmannite(1)	-68.50	-58.00	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-63.28	-45.28	18.00	Fe8O8(OH)6SO4
Sepiolite	-5.15	10.72	15.86	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-7.94	10.72	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-2.26	-13.12	-10.87	FeCO3
SiO2(a)	-0.85	-3.60	-2.74	SiO2
Sulfur	-2.54	2.44	4.97	S
Talc	-3.96	17.88	21.84	Mg3Si4O10(OH)2
Troilite	-0.40	-6.55	-6.15	FeS
Witherite	-3.14	-11.71	-8.57	BaCO3

End of simulation.

Reading input data for simulation 6.

SOLUTION 1 BB05D 9-6-2007

temp	21.8
pH	6.61
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Fe	0.75
S(6)	1040 as SO4
S(-2)	0.01
Cl	465
Br	2.56
Alkalinity	850 as HCO3
Ba	0.03
Ca	237
Mg	146
Na	606
K	3.53
Mn	0.83
Si	11.1
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. BB05D 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.393e-002	1.393e-002
Ba	2.184e-007	2.184e-007
Br	3.204e-005	3.204e-005
Ca	5.913e-003	5.913e-003
Cl	1.312e-002	1.312e-002
Fe	1.343e-005	1.343e-005
K	9.028e-005	9.028e-005
Mg	6.005e-003	6.005e-003
Mn	1.511e-005	1.511e-005
Na	2.636e-002	2.636e-002
S(-2)	3.119e-007	3.119e-007
S(6)	1.083e-002	1.083e-002
Si	1.847e-004	1.847e-004

-----Description of solution-----

pH	=	6.610
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	5.919e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	2.005e-002
Total CO2 (mol/kg)	=	2.005e-002
Temperature (deg C)	=	21.800
Electrical balance (eq)	=	1.614e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	1.88
Iterations	=	9
Total H	=	1.110271e+002
Total O	=	5.560427e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.5948	-0.1518

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.896e-007	2.455e-007	-6.538	-6.610	-0.072
OH-	3.975e-008	3.184e-008	-7.401	-7.497	-0.096
H2O	5.551e+001	9.987e-001	1.744	-0.001	0.000
Ba	2.184e-007				
Ba+2	1.216e-007	5.400e-008	-6.915	-7.268	-0.352
BaSO4	9.059e-008	9.184e-008	-7.043	-7.037	0.006
BaHCO3+	6.211e-009	5.047e-009	-8.207	-8.297	-0.090

BaCO3	4.971e-011	5.039e-011	-10.304	-10.298	0.006
BaOH+	9.162e-015	7.445e-015	-14.038	-14.128	-0.090
Br	3.204e-005				
Br-	3.204e-005	2.548e-005	-4.494	-4.594	-0.099
C (4)	2.005e-002				
HCO3-	1.315e-002	1.078e-002	-1.881	-1.967	-0.086
CO2	6.133e-003	6.217e-003	-2.212	-2.206	0.006
CaHCO3+	3.126e-004	2.564e-004	-3.505	-3.591	-0.086
MgHCO3+	3.048e-004	2.477e-004	-3.516	-3.606	-0.090
NaHCO3	1.257e-004	1.275e-004	-3.901	-3.895	0.006
CaCO3	5.899e-006	5.980e-006	-5.229	-5.223	0.006
MnHCO3+	4.357e-006	3.540e-006	-5.361	-5.451	-0.090
FeHCO3+	4.335e-006	3.522e-006	-5.363	-5.453	-0.090
CO3-2	4.258e-006	1.926e-006	-5.371	-5.715	-0.345
MgCO3	3.433e-006	3.480e-006	-5.464	-5.458	0.006
NaCO3-	7.881e-007	6.404e-007	-6.103	-6.194	-0.090
MnCO3	5.559e-007	5.636e-007	-6.255	-6.249	0.006
FeCO3	1.489e-007	1.509e-007	-6.827	-6.821	0.006
BaHCO3+	6.211e-009	5.047e-009	-8.207	-8.297	-0.090
Fe (CO3) (OH) -	2.940e-009	2.389e-009	-8.532	-8.622	-0.090
Fe (CO3) 2-2	7.834e-010	3.415e-010	-9.106	-9.467	-0.361
BaCO3	4.971e-011	5.039e-011	-10.304	-10.298	0.006
Ca	5.913e-003				
Ca+2	4.322e-003	1.964e-003	-2.364	-2.707	-0.343
CaSO4	1.272e-003	1.290e-003	-2.895	-2.889	0.006
CaHCO3+	3.126e-004	2.564e-004	-3.505	-3.591	-0.086
CaCO3	5.899e-006	5.980e-006	-5.229	-5.223	0.006
CaHSO4+	2.196e-009	1.784e-009	-8.658	-8.749	-0.090
CaOH+	1.632e-009	1.326e-009	-8.787	-8.878	-0.090
Cl	1.312e-002				
Cl-	1.312e-002	1.053e-002	-1.882	-1.978	-0.095
MnCl+	1.944e-007	1.580e-007	-6.711	-6.801	-0.090
FeCl+	5.842e-008	4.747e-008	-7.233	-7.324	-0.090
MnCl2	7.162e-010	7.260e-010	-9.145	-9.139	0.006
MnCl3-	2.591e-012	2.105e-012	-11.587	-11.677	-0.090
FeCl+2	4.372e-022	1.906e-022	-21.359	-21.720	-0.361
FeCl2+	1.222e-023	9.932e-024	-22.913	-23.003	-0.090
FeCl3	1.031e-026	1.046e-026	-25.987	-25.981	0.006
Fe (2)	1.343e-005				
Fe+2	7.040e-006	3.267e-006	-5.152	-5.486	-0.333
FeHCO3+	4.335e-006	3.522e-006	-5.363	-5.453	-0.090
FeSO4	1.833e-006	1.858e-006	-5.737	-5.731	0.006
FeCO3	1.489e-007	1.509e-007	-6.827	-6.821	0.006
FeCl+	5.842e-008	4.747e-008	-7.233	-7.324	-0.090
FeS	7.041e-009	7.138e-009	-8.152	-8.146	0.006
FeOH+	4.062e-009	3.300e-009	-8.391	-8.481	-0.090
Fe (CO3) (OH) -	2.940e-009	2.389e-009	-8.532	-8.622	-0.090
Fe (CO3) 2-2	7.834e-010	3.415e-010	-9.106	-9.467	-0.361
Fe (HS) 2	2.075e-011	2.104e-011	-10.683	-10.677	0.006
FeHSO4+	3.653e-012	2.969e-012	-11.437	-11.527	-0.090
Fe (OH) 2	1.309e-013	1.327e-013	-12.883	-12.877	0.006
Fe (HS) 3-	2.396e-016	1.947e-016	-15.620	-15.711	-0.090
Fe (3)	2.893e-014				
Fe (OH) 2+	2.115e-014	1.719e-014	-13.675	-13.765	-0.090

Fe (OH) 3	7.718e-015	7.823e-015	-14.113	-14.107	0.006
FeOH+2	3.308e-017	1.442e-017	-16.480	-16.841	-0.361
Fe (OH) 4-	3.137e-017	2.549e-017	-16.504	-16.594	-0.090
FeSO4+	2.831e-020	2.301e-020	-19.548	-19.638	-0.090
Fe+3	2.938e-021	6.643e-022	-20.532	-21.178	-0.646
Fe (SO4) 2-	2.075e-021	1.686e-021	-20.683	-20.773	-0.090
FeCl+2	4.372e-022	1.906e-022	-21.359	-21.720	-0.361
FeCl2+	1.222e-023	9.932e-024	-22.913	-23.003	-0.090
FeHSO4+2	3.478e-026	1.516e-026	-25.459	-25.819	-0.361
FeCl3	1.031e-026	1.046e-026	-25.987	-25.981	0.006
Fe2 (OH) 2+4	1.772e-031	6.400e-033	-30.752	-32.194	-1.442
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-41.256	-43.509	-2.253
H (0)	1.345e-011				
H2	6.724e-012	6.816e-012	-11.172	-11.166	0.006
K	9.028e-005				
K+	8.831e-005	7.088e-005	-4.054	-4.149	-0.095
KSO4-	1.966e-006	1.597e-006	-5.707	-5.797	-0.090
KOH	9.864e-013	9.999e-013	-12.006	-12.000	0.006
Mg	6.005e-003				
Mg+2	4.261e-003	1.989e-003	-2.370	-2.701	-0.331
MgSO4	1.436e-003	1.456e-003	-2.843	-2.837	0.006
MgHCO3+	3.048e-004	2.477e-004	-3.516	-3.606	-0.090
MgCO3	3.433e-006	3.480e-006	-5.464	-5.458	0.006
MgOH+	1.165e-008	9.467e-009	-7.934	-8.024	-0.090
Mn (2)	1.511e-005				
Mn+2	7.938e-006	3.684e-006	-5.100	-5.434	-0.333
MnHCO3+	4.357e-006	3.540e-006	-5.361	-5.451	-0.090
MnSO4	2.061e-006	2.090e-006	-5.686	-5.680	0.006
MnCO3	5.559e-007	5.636e-007	-6.255	-6.249	0.006
MnCl+	1.944e-007	1.580e-007	-6.711	-6.801	-0.090
MnCl2	7.162e-010	7.260e-010	-9.145	-9.139	0.006
MnOH+	3.642e-010	2.959e-010	-9.439	-9.529	-0.090
MnCl3-	2.591e-012	2.105e-012	-11.587	-11.677	-0.090
Mn (3)	1.168e-033				
Mn+3	1.168e-033	1.804e-034	-32.932	-33.744	-0.811
Na	2.636e-002				
Na+	2.580e-002	2.102e-002	-1.588	-1.677	-0.089
NaSO4-	4.310e-004	3.502e-004	-3.366	-3.456	-0.090
NaHCO3	1.257e-004	1.275e-004	-3.901	-3.895	0.006
NaCO3-	7.881e-007	6.404e-007	-6.103	-6.194	-0.090
NaOH	5.574e-010	5.650e-010	-9.254	-9.248	0.006
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-71.098	-71.092	0.006
S (-2)	3.119e-007				
H2S	1.987e-007	2.014e-007	-6.702	-6.696	0.006
HS-	1.061e-007	8.500e-008	-6.974	-7.071	-0.096
FeS	7.041e-009	7.138e-009	-8.152	-8.146	0.006
Fe (HS) 2	2.075e-011	2.104e-011	-10.683	-10.677	0.006
S-2	7.545e-014	3.351e-014	-13.122	-13.475	-0.352
Fe (HS) 3-	2.396e-016	1.947e-016	-15.620	-15.711	-0.090
S (6)	1.083e-002				
SO4-2	7.681e-003	3.393e-003	-2.115	-2.469	-0.355
MgSO4	1.436e-003	1.456e-003	-2.843	-2.837	0.006
CaSO4	1.272e-003	1.290e-003	-2.895	-2.889	0.006

NaSO4-	4.310e-004	3.502e-004	-3.366	-3.456	-0.090
MnSO4	2.061e-006	2.090e-006	-5.686	-5.680	0.006
KSO4-	1.966e-006	1.597e-006	-5.707	-5.797	-0.090
FeSO4	1.833e-006	1.858e-006	-5.737	-5.731	0.006
HSO4-	9.302e-008	7.559e-008	-7.031	-7.122	-0.090
BaSO4	9.059e-008	9.184e-008	-7.043	-7.037	0.006
CaHSO4+	2.196e-009	1.784e-009	-8.658	-8.749	-0.090
FeHSO4+	3.653e-012	2.969e-012	-11.437	-11.527	-0.090
FeSO4+	2.831e-020	2.301e-020	-19.548	-19.638	-0.090
Fe (SO4) 2-	2.075e-021	1.686e-021	-20.683	-20.773	-0.090
FeHSO4+2	3.478e-026	1.516e-026	-25.459	-25.819	-0.361
Si	1.847e-004				
H4SiO4	1.846e-004	1.872e-004	-3.734	-3.728	0.006
H3SiO4-	1.235e-007	1.003e-007	-6.908	-6.999	-0.090
H2SiO4-2	5.157e-014	2.249e-014	-13.288	-13.648	-0.361

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-3.61	19.48	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	2.22	27.21	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-10.89	31.23	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-22.86	35.49	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-21.64	38.74	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-17.20	26.36	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-0.83	-5.18	-4.35	CaSO4
Aragonite	-0.11	-8.42	-8.32	CaCO3
Barite	0.29	-9.74	-10.02	BaSO4
Brucite	-6.27	10.52	16.79	Mg (OH) 2
Calcite	0.04	-8.42	-8.46	CaCO3
Chalcedony	-0.14	-3.73	-3.59	SiO2
Chrysotile	-8.50	24.10	32.60	Mg3Si2O5 (OH) 4
CO2 (g)	-0.78	-2.21	-1.43	CO2
Dolomite	0.18	-16.84	-17.01	CaMg (CO3) 2
Epsomite	-3.01	-5.17	-2.16	MgSO4:7H2O
Fe (OH) 2 (1)	-5.21	7.73	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-6.16	7.73	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-6.24	-1.35	4.89	Fe (OH) 3
FeO	-5.86	7.73	13.59	FeO
FeS (am)	-2.07	-5.95	-3.88	FeS
FeS (ppt)	-2.03	-5.95	-3.92	FeS
Goethite	-0.46	-1.35	-0.88	FeOOH
Greigite	-10.98	-49.68	-38.70	Fe3S4
Gypsum	-0.60	-5.18	-4.58	CaSO4:2H2O
H2 (g)	-8.03	-11.17	-3.14	H2
H2O (g)	-1.59	-0.00	1.59	H2O
H2S (g)	-5.74	-6.70	-0.96	H2S
Halite	-5.23	-3.66	1.57	NaCl
Hausmannite	-30.44	31.39	61.83	Mn3O4
Hematite	1.07	-2.70	-3.76	Fe2O3
Jarosite-H3O	-23.75	-35.43	-11.67	H3OFe3 (SO4) 2 (OH) 6
Jarosite-K	-22.05	-32.96	-10.91	KFe3 (SO4) 2 (OH) 6
Lepidocrocite	-4.95	11.75	16.70	FeOOH

Lime	-12.30	10.51	22.81	Ca (OH) 2
Mackinawite	-1.33	-5.95	-4.61	FeS
Mackinawite(2)	-2.46	1.04	3.50	FeS
Magnetite	-14.57	31.23	45.80	Fe3O4
Manganite	-13.54	11.80	25.34	MnOOH
Marcasite	6.25	-11.60	-17.85	FeS2
Melanterite	-5.71	-7.96	-2.25	FeSO4:7H2O
Nesquehonite	-2.84	-8.42	-5.57	MgCO3:3H2O
O2(g)	-68.15	-71.09	-2.95	O2
Pyrite	6.97	-11.60	-18.57	FeS2
Pyrochroite	-7.41	7.79	15.20	Mn (OH) 2
Pyrolusite	-26.08	15.82	41.90	MnO2
Quartz	0.30	-3.73	-4.03	SiO2
Rhodochrosite	-0.03	-11.15	-11.12	MnCO3
Schwertmannite(1)	-49.53	-39.03	10.50	Fe8O8(OH) 4.4 (SO4) 1.8:8.4H2O
Schwertmannite(2)	-44.48	-26.48	18.00	Fe8O8(OH) 6SO4
Sepiolite	-5.99	9.85	15.85	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-8.81	9.85	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-0.33	-11.20	-10.87	FeCO3
SiO2(a)	-0.99	-3.73	-2.74	SiO2
Sulfur	-3.62	1.33	4.96	S
Talc	-5.12	16.65	21.77	Mg3Si4O10(OH) 2
Troilite	0.21	-5.95	-6.15	FeS
Witherite	-4.41	-12.98	-8.57	BaCO3

End of simulation.

Reading input data for simulation 7.

SOLUTION 1 EPAUMP1 9-6-2007

temp	21.8
pH	6.96
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Fe	0.5
S(6)	2040 as SO4
S(-2)	0.005
Cl	336
Br	1.5
Alkalinity	240 as HCO3
Ba	0.009
Ca	530
Mg	129
Na	445
K	5.78
Mn	0.11
Si	7.3
Sr	6.70

Zn 0.067
water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. EPAUMP1 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	3.933e-003	3.933e-003
Ba	6.553e-008	6.553e-008
Br	1.877e-005	1.877e-005
Ca	1.322e-002	1.322e-002
Cl	9.477e-003	9.477e-003
Fe	8.953e-006	8.953e-006
K	1.478e-004	1.478e-004
Mg	5.306e-003	5.306e-003
Mn	2.002e-006	2.002e-006
Na	1.936e-002	1.936e-002
S(-2)	1.559e-007	1.559e-007
S(6)	2.124e-002	2.124e-002
Si	1.215e-004	1.215e-004
Sr	7.647e-005	7.647e-005
Zn	1.025e-006	1.025e-006

-----Description of solution-----

pH	=	6.960
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	6.931e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	4.672e-003
Total CO2 (mol/kg)	=	4.672e-003
Temperature (deg C)	=	21.800
Electrical balance (eq)	=	8.394e-004
Percent error, 100*(Cat- An)/(Cat+ An)	=	0.98
Iterations	=	10
Total H	=	1.110168e+002
Total O	=	5.560491e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.9415	-0.1721

-----Distribution of species-----

Log	Log	Log
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Species	Molality	Activity	Molality	Activity	Gamma
H+	1.303e-007	1.096e-007	-6.885	-6.960	-0.075
OH-	9.026e-008	7.130e-008	-7.045	-7.147	-0.102
H2O	5.551e+001	9.989e-001	1.744	-0.000	0.000
Ba	6.553e-008				
BaSO4	3.638e-008	3.697e-008	-7.439	-7.432	0.007
Ba+2	2.875e-008	1.219e-008	-7.541	-7.914	-0.373
BaHCO3+	3.894e-010	3.129e-010	-9.410	-9.505	-0.095
BaCO3	6.882e-012	6.993e-012	-11.162	-11.155	0.007
BaOH+	4.683e-015	3.763e-015	-14.329	-14.425	-0.095
Br	1.877e-005				
Br-	1.877e-005	1.471e-005	-4.726	-4.832	-0.106
C (4)	4.672e-003				
HCO3-	3.652e-003	2.961e-003	-2.438	-2.528	-0.091
CO2	7.505e-004	7.626e-004	-3.125	-3.118	0.007
CaHCO3+	1.672e-004	1.356e-004	-3.777	-3.868	-0.091
MgHCO3+	6.351e-005	5.103e-005	-4.197	-4.292	-0.095
NaHCO3	2.478e-005	2.518e-005	-4.606	-4.599	0.007
CaCO3	6.970e-006	7.082e-006	-5.157	-5.150	0.007
CO3-2	2.737e-006	1.184e-006	-5.563	-5.927	-0.364
MgCO3	1.580e-006	1.605e-006	-5.801	-5.794	0.007
SrHCO3+	1.109e-006	8.994e-007	-5.955	-6.046	-0.091
FeHCO3+	9.012e-007	7.241e-007	-6.045	-6.140	-0.095
NaCO3-	3.525e-007	2.832e-007	-6.453	-6.548	-0.095
MnHCO3+	1.777e-007	1.428e-007	-6.750	-6.845	-0.095
ZnHCO3+	1.027e-007	8.250e-008	-6.988	-7.084	-0.095
FeCO3	6.836e-008	6.946e-008	-7.165	-7.158	0.007
ZnCO3	5.146e-008	5.229e-008	-7.289	-7.282	0.007
MnCO3	5.008e-008	5.088e-008	-7.300	-7.293	0.007
SrCO3	1.500e-008	1.524e-008	-7.824	-7.817	0.007
Zn (CO3) 2-2	3.177e-009	1.324e-009	-8.498	-8.878	-0.380
Fe (CO3) (OH) -	3.064e-009	2.462e-009	-8.514	-8.609	-0.095
BaHCO3+	3.894e-010	3.129e-010	-9.410	-9.505	-0.095
Fe (CO3) 2-2	2.319e-010	9.664e-011	-9.635	-10.015	-0.380
BaCO3	6.882e-012	6.993e-012	-11.162	-11.155	0.007
Ca	1.322e-002				
Ca+2	8.689e-003	3.782e-003	-2.061	-2.422	-0.361
CaSO4	4.361e-003	4.431e-003	-2.360	-2.354	0.007
CaHCO3+	1.672e-004	1.356e-004	-3.777	-3.868	-0.091
CaCO3	6.970e-006	7.082e-006	-5.157	-5.150	0.007
CaOH+	7.117e-009	5.718e-009	-8.148	-8.243	-0.095
CaHSO4+	3.408e-009	2.738e-009	-8.468	-8.563	-0.095
Cl	9.477e-003				
Cl-	9.477e-003	7.504e-003	-2.023	-2.125	-0.101
FeCl+	3.152e-008	2.533e-008	-7.501	-7.596	-0.095
MnCl+	2.058e-008	1.654e-008	-7.687	-7.782	-0.095
ZnCl+	4.823e-009	3.875e-009	-8.317	-8.412	-0.095
MnCl2	5.331e-011	5.417e-011	-10.273	-10.266	0.007
ZnCl2	2.958e-011	3.006e-011	-10.529	-10.522	0.007
ZnCl3-	3.089e-013	2.482e-013	-12.510	-12.605	-0.095
MnCl3-	1.393e-013	1.120e-013	-12.856	-12.951	-0.095
ZnCl4-2	2.183e-015	9.099e-016	-14.661	-15.041	-0.380
FeCl+2	1.098e-022	4.576e-023	-21.959	-22.339	-0.380

FeCl ₂ +	2.115e-024	1.700e-024	-23.675	-23.770	-0.095
FeCl ₃	1.255e-027	1.275e-027	-26.901	-26.894	0.007
Fe (2)	8.953e-006				
Fe+2	5.492e-006	2.445e-006	-5.260	-5.612	-0.351
FeSO ₄	2.441e-006	2.480e-006	-5.612	-5.606	0.007
FeHCO ₃ +	9.012e-007	7.241e-007	-6.045	-6.140	-0.095
FeCO ₃	6.836e-008	6.946e-008	-7.165	-7.158	0.007
FeCl+	3.152e-008	2.533e-008	-7.501	-7.596	-0.095
FeS	8.826e-009	8.968e-009	-8.054	-8.047	0.007
FeOH+	6.884e-009	5.531e-009	-8.162	-8.257	-0.095
Fe (CO ₃) (OH) -	3.064e-009	2.462e-009	-8.514	-8.609	-0.095
Fe (CO ₃) 2-2	2.319e-010	9.664e-011	-9.635	-10.015	-0.380
Fe (HS) 2	8.714e-012	8.854e-012	-11.060	-11.053	0.007
FeHSO ₄ +	2.203e-012	1.770e-012	-11.657	-11.752	-0.095
Fe (OH) 2	4.902e-013	4.981e-013	-12.310	-12.303	0.007
Fe (HS) 3-	7.649e-017	6.146e-017	-16.116	-16.211	-0.095
Fe (3)	6.554e-014				
Fe (OH) 2+	3.613e-014	2.903e-014	-13.442	-13.537	-0.095
Fe (OH) 3	2.912e-014	2.958e-014	-13.536	-13.529	0.007
Fe (OH) 4-	2.686e-016	2.158e-016	-15.571	-15.666	-0.095
FeOH+2	2.610e-017	1.088e-017	-16.583	-16.963	-0.380
FeSO ₄ +	1.720e-020	1.382e-020	-19.764	-19.859	-0.095
Fe (SO ₄) 2-	2.249e-021	1.807e-021	-20.648	-20.743	-0.095
Fe+3	1.060e-021	2.237e-022	-20.975	-21.650	-0.676
FeCl+2	1.098e-022	4.576e-023	-21.959	-22.339	-0.380
FeCl ₂ +	2.115e-024	1.700e-024	-23.675	-23.770	-0.095
FeHSO ₄ +2	9.764e-027	4.069e-027	-26.010	-26.391	-0.380
FeCl ₃	1.255e-027	1.275e-027	-26.901	-26.894	0.007
Fe ₂ (OH) 2+4	1.207e-031	3.640e-033	-30.918	-32.439	-1.521
Fe ₃ (OH) 4+5	0.000e+000	0.000e+000	-41.150	-43.526	-2.376
H (0)	1.322e-011				
H ₂	6.609e-012	6.715e-012	-11.180	-11.173	0.007
K	1.478e-004				
K+	1.422e-004	1.126e-004	-3.847	-3.949	-0.101
KSO ₄ -	5.631e-006	4.525e-006	-5.249	-5.344	-0.095
KOH	3.500e-012	3.556e-012	-11.456	-11.449	0.007
Mg	5.306e-003				
Mg+2	3.324e-003	1.492e-003	-2.478	-2.826	-0.348
MgSO ₄	1.917e-003	1.948e-003	-2.717	-2.711	0.007
MgHCO ₃ +	6.351e-005	5.103e-005	-4.197	-4.292	-0.095
MgCO ₃	1.580e-006	1.605e-006	-5.801	-5.794	0.007
MgOH+	1.979e-008	1.590e-008	-7.704	-7.799	-0.095
Mn (2)	2.002e-006				
Mn+2	1.215e-006	5.409e-007	-5.915	-6.267	-0.351
MnSO ₄	5.386e-007	5.473e-007	-6.269	-6.262	0.007
MnHCO ₃ +	1.777e-007	1.428e-007	-6.750	-6.845	-0.095
MnCO ₃	5.008e-008	5.088e-008	-7.300	-7.293	0.007
MnCl+	2.058e-008	1.654e-008	-7.687	-7.782	-0.095
MnOH+	1.211e-010	9.730e-011	-9.917	-10.012	-0.095
MnCl ₂	5.331e-011	5.417e-011	-10.273	-10.266	0.007
MnCl ₃ -	1.393e-013	1.120e-013	-12.856	-12.951	-0.095
Mn (3)	8.546e-035				
Mn+3	8.546e-035	1.192e-035	-34.068	-34.924	-0.855
Na	1.936e-002				

Na+	1.877e-002	1.512e-002	-1.726	-1.820	-0.094
NaSO4-	5.592e-004	4.493e-004	-3.252	-3.347	-0.095
NaHCO3	2.478e-005	2.518e-005	-4.606	-4.599	0.007
NaCO3-	3.525e-007	2.832e-007	-6.453	-6.548	-0.095
NaOH	8.957e-010	9.101e-010	-9.048	-9.041	0.007
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-71.086	-71.079	0.007
S (-2)	1.559e-007				
HS-	8.070e-008	6.374e-008	-7.093	-7.196	-0.102
H2S	6.640e-008	6.746e-008	-7.178	-7.171	0.007
FeS	8.826e-009	8.968e-009	-8.054	-8.047	0.007
Fe (HS) 2	8.714e-012	8.854e-012	-11.060	-11.053	0.007
S-2	1.327e-013	5.626e-014	-12.877	-13.250	-0.373
Fe (HS) 3-	7.649e-017	6.146e-017	-16.116	-16.211	-0.095
S (6)	2.124e-002				
SO4-2	1.437e-002	6.052e-003	-1.843	-2.218	-0.375
CaSO4	4.361e-003	4.431e-003	-2.360	-2.354	0.007
MgSO4	1.917e-003	1.948e-003	-2.717	-2.711	0.007
NaSO4-	5.592e-004	4.493e-004	-3.252	-3.347	-0.095
SrSO4	2.477e-005	2.516e-005	-4.606	-4.599	0.007
KSO4-	5.631e-006	4.525e-006	-5.249	-5.344	-0.095
FeSO4	2.441e-006	2.480e-006	-5.612	-5.606	0.007
MnSO4	5.386e-007	5.473e-007	-6.269	-6.262	0.007
ZnSO4	3.014e-007	3.062e-007	-6.521	-6.514	0.007
HSO4-	7.495e-008	6.022e-008	-7.125	-7.220	-0.095
Zn (SO4) 2-2	3.706e-008	1.544e-008	-7.431	-7.811	-0.380
BaSO4	3.638e-008	3.697e-008	-7.439	-7.432	0.007
CaHSO4+	3.408e-009	2.738e-009	-8.468	-8.563	-0.095
FeHSO4+	2.203e-012	1.770e-012	-11.657	-11.752	-0.095
FeSO4+	1.720e-020	1.382e-020	-19.764	-19.859	-0.095
Fe (SO4) 2-	2.249e-021	1.807e-021	-20.648	-20.743	-0.095
FeHSO4+2	9.764e-027	4.069e-027	-26.010	-26.391	-0.380
Si	1.215e-004				
H4SiO4	1.213e-004	1.233e-004	-3.916	-3.909	0.007
H3SiO4-	1.841e-007	1.480e-007	-6.735	-6.830	-0.095
H2SiO4-2	1.781e-013	7.422e-014	-12.749	-13.129	-0.380
Sr	7.647e-005				
Sr+2	5.058e-005	2.215e-005	-4.296	-4.655	-0.359
SrSO4	2.477e-005	2.516e-005	-4.606	-4.599	0.007
SrHCO3+	1.109e-006	8.994e-007	-5.955	-6.046	-0.091
SrCO3	1.500e-008	1.524e-008	-7.824	-7.817	0.007
SrOH+	1.283e-011	1.035e-011	-10.892	-10.985	-0.093
Zn	1.025e-006				
Zn+2	5.219e-007	2.213e-007	-6.282	-6.655	-0.373
ZnSO4	3.014e-007	3.062e-007	-6.521	-6.514	0.007
ZnHCO3+	1.027e-007	8.250e-008	-6.988	-7.084	-0.095
ZnCO3	5.146e-008	5.229e-008	-7.289	-7.282	0.007
Zn (SO4) 2-2	3.706e-008	1.544e-008	-7.431	-7.811	-0.380
ZnCl+	4.823e-009	3.875e-009	-8.317	-8.412	-0.095
Zn (CO3) 2-2	3.177e-009	1.324e-009	-8.498	-8.878	-0.380
ZnOH+	2.153e-009	1.729e-009	-8.667	-8.762	-0.095
Zn (OH) 2	2.275e-010	2.312e-010	-9.643	-9.636	0.007
ZnCl2	2.958e-011	3.006e-011	-10.529	-10.522	0.007
ZnCl3-	3.089e-013	2.482e-013	-12.510	-12.605	-0.095

Zn(OH) 3-	8.290e-015	6.660e-015	-14.081	-14.177	-0.095
ZnCl4-2	2.183e-015	9.099e-016	-14.661	-15.041	-0.380
Zn(OH) 4-2	2.308e-020	9.616e-021	-19.637	-20.017	-0.380

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH) 5]	-2.46	20.63	23.09	Fe2(OH) 5
[Fe3(OH) 7]	3.95	28.94	24.99	Fe3(OH) 7
[Fe3(OH) 8]	-9.16	32.96	42.12	Fe3(OH) 8
[Fe6(OH) 12] [CO3]	-20.32	38.03	58.35	Fe6(OH) 12 (CO3) 1
[Fe6(OH) 12] [SO4]	-18.64	41.74	60.38	Fe6(OH) 12 (SO4) 1
[Fe6(OH) 8] [Cl]	-15.40	28.16	43.56	Fe4(OH) 8 (Cl) 1
Anhydrite	-0.29	-4.64	-4.35	CaSO4
Aragonite	-0.03	-8.35	-8.32	CaCO3
Barite	-0.11	-10.13	-10.02	BaSO4
Brucite	-5.70	11.09	16.79	Mg(OH) 2
Calcite	0.11	-8.35	-8.46	CaCO3
Celestite	-0.25	-6.87	-6.63	SrSO4
Chalcedony	-0.32	-3.91	-3.59	SiO2
Chrysotile	-7.14	25.46	32.60	Mg3Si2O5(OH) 4
CO2(g)	-1.69	-3.12	-1.43	CO2
Dolomite	-0.09	-17.10	-17.01	CaMg(CO3) 2
Epsomite	-2.89	-5.05	-2.16	MgSO4:7H2O
Fe(OH) 2 (1)	-4.63	8.31	12.94	Fe(OH) 2
Fe(OH) 2 (2)	-5.58	8.31	13.89	Fe(OH) 2
Fe(OH) 3 (a)	-5.66	-0.77	4.89	Fe(OH) 3
FeO	-5.28	8.31	13.59	FeO
FeS(am)	-1.97	-5.85	-3.88	FeS
FeS(ppt)	-1.93	-5.85	-3.92	FeS
Goethite	0.11	-0.77	-0.88	FeOOH
Greigite	-11.16	-49.85	-38.70	Fe3S4
Gypsum	-0.06	-4.64	-4.58	CaSO4:2H2O
H2(g)	-8.04	-11.17	-3.14	H2
H2O(g)	-1.59	-0.00	1.59	H2O
H2S(g)	-6.21	-7.17	-0.96	H2S
Halite	-5.52	-3.95	1.57	NaCl
Hausmannite	-30.84	30.99	61.83	Mn3O4
Hematite	2.22	-1.54	-3.76	Fe2O3
Jarosite-H3O	-22.92	-34.59	-11.67	H3OFe3(SO4) 2 (OH) 6
Jarosite-K	-20.66	-31.58	-10.91	KFe3(SO4) 2 (OH) 6
Lepidocrocite	-4.37	12.33	16.70	FeOOH
Lime	-11.31	11.50	22.81	Ca(OH) 2
Mackinawite	-1.23	-5.85	-4.61	FeS
Mackinawite(2)	-2.36	1.14	3.50	FeS
Magnetite	-12.84	32.96	45.80	Fe3O4
Manganite	-13.67	11.67	25.34	MnOOH
Marcasite	5.88	-11.97	-17.85	FeS2
Melanterite	-5.58	-7.83	-2.25	FeSO4:7H2O
Nesquehonite	-3.18	-8.75	-5.57	MgCO3:3H2O
O2(g)	-68.13	-71.08	-2.95	O2
Pyrite	6.60	-11.97	-18.57	FeS2
Pyrochroite	-7.55	7.65	15.20	Mn(OH) 2

Pyrolusite	-26.21	15.69	41.90	MnO2
Quartz	0.12	-3.91	-4.03	SiO2
Rhodochrosite	-1.07	-12.19	-11.12	MnCO3
Schwertmannite(1)	-45.72	-35.22	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-40.31	-22.31	18.00	Fe8O8(OH)6SO4
Sepiolite	-5.38	10.46	15.85	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-8.20	10.46	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-0.67	-11.54	-10.87	FeCO3
SiO2(a)	-1.17	-3.91	-2.74	SiO2
Smithsonite	-2.62	-12.58	-9.97	ZnCO3
Sphalerite	4.79	-6.89	-11.68	ZnS
Strontianite	-1.31	-10.58	-9.27	SrCO3
Sulfur	-4.09	0.87	4.96	S
Talc	-4.12	17.65	21.77	Mg3Si4O10(OH)2
Troilite	0.31	-5.85	-6.15	FeS
Willemite	-4.97	10.62	15.60	Zn2SiO4
Witherite	-5.27	-13.84	-8.57	BaCO3
Zn(OH)2(e)	-4.24	7.26	11.50	Zn(OH)2

End of simulation.

Reading input data for simulation 8.

SOLUTION 1 MP1 9-6-2007

temp	20.3
pH	6.43
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Fe	0.4
S(6)	145 as SO4
S(-2)	0.39
Cl	267
Br	0.44
Alkalinity 2000 as HCO3	
Ba	0.72
Ca	366
Mg	114
Na	334
K	25.9
Mn	1.6
Si	17.8
Sr	4.76
Zn	0.133
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. MP1 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	3.278e-002	3.278e-002
Ba	5.242e-006	5.242e-006
Br	5.507e-006	5.507e-006
Ca	9.132e-003	9.132e-003
Cl	7.531e-003	7.531e-003
Fe	7.162e-006	7.162e-006
K	6.624e-004	6.624e-004
Mg	4.689e-003	4.689e-003
Mn	2.912e-005	2.912e-005
Na	1.453e-002	1.453e-002
S(-2)	1.216e-005	1.216e-005
S(6)	1.509e-003	1.509e-003
Si	2.963e-004	2.963e-004
Sr	5.433e-005	5.433e-005
Zn	2.035e-006	2.035e-006

-----Description of solution-----

pH	=	6.430
pe	=	4.000
Activity of water	=	0.998
Ionic strength	=	5.247e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	5.505e-002
Total CO2 (mol/kg)	=	5.505e-002
Temperature (deg C)	=	20.300
Electrical balance (eq)	=	-3.042e-004
Percent error, 100*(Cat- An)/(Cat+ An)	=	-0.38
Iterations	=	10
Total H	=	1.110464e+002
Total O	=	5.565629e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.6550	-0.1546

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	4.356e-007	3.715e-007	-6.361	-6.430	-0.069
OH-	2.308e-008	1.869e-008	-7.637	-7.728	-0.092
H2O	5.551e+001	9.985e-001	1.744	-0.001	0.000
Ba	5.242e-006				

Ba+2	4.290e-006	1.976e-006	-5.368	-5.704	-0.337
BaHCO3+	5.041e-007	4.133e-007	-6.298	-6.384	-0.086
BaSO4	4.462e-007	4.516e-007	-6.350	-6.345	0.005
BaCO3	2.650e-009	2.682e-009	-8.577	-8.572	0.005
BaOH+	2.194e-013	1.799e-013	-12.659	-12.745	-0.086
Br	5.507e-006				
Br-	5.507e-006	4.430e-006	-5.259	-5.354	-0.094
C (4)	5.505e-002				
HCO3-	3.059e-002	2.530e-002	-1.514	-1.597	-0.082
CO2	2.231e-002	2.258e-002	-1.652	-1.646	0.005
CaHCO3+	1.276e-003	1.056e-003	-2.894	-2.976	-0.082
MgHCO3+	6.578e-004	5.393e-004	-3.182	-3.268	-0.086
NaHCO3	1.656e-004	1.676e-004	-3.781	-3.776	0.005
CaCO3	1.557e-005	1.576e-005	-4.808	-4.802	0.005
MnHCO3+	1.550e-005	1.271e-005	-4.810	-4.896	-0.086
SrHCO3+	8.325e-006	6.886e-006	-5.080	-5.162	-0.082
CO3-2	6.167e-006	2.888e-006	-5.210	-5.539	-0.330
MgCO3	4.701e-006	4.758e-006	-5.328	-5.323	0.005
FeHCO3+	4.114e-006	3.373e-006	-5.386	-5.472	-0.086
MnCO3	1.278e-006	1.293e-006	-5.894	-5.888	0.005
ZnHCO3+	1.158e-006	9.495e-007	-5.936	-6.023	-0.086
NaCO3-	6.072e-007	4.979e-007	-6.217	-6.303	-0.086
BaHCO3+	5.041e-007	4.133e-007	-6.298	-6.384	-0.086
ZnCO3	1.697e-007	1.717e-007	-6.770	-6.765	0.005
FeCO3	9.125e-008	9.236e-008	-7.040	-7.035	0.005
SrCO3	3.313e-008	3.353e-008	-7.480	-7.475	0.005
Zn (CO3) 2-2	2.346e-008	1.060e-008	-7.630	-7.975	-0.345
BaCO3	2.650e-009	2.682e-009	-8.577	-8.572	0.005
Fe (CO3) (OH) -	1.178e-009	9.656e-010	-8.929	-9.015	-0.086
Fe (CO3) 2-2	6.933e-010	3.134e-010	-9.159	-9.504	-0.345
Ca	9.132e-003				
Ca+2	7.535e-003	3.541e-003	-2.123	-2.451	-0.328
CaHCO3+	1.276e-003	1.056e-003	-2.894	-2.976	-0.082
CaSO4	3.044e-004	3.081e-004	-3.516	-3.511	0.005
CaCO3	1.557e-005	1.576e-005	-4.808	-4.802	0.005
CaOH+	1.926e-009	1.579e-009	-8.715	-8.802	-0.086
CaHSO4+	7.735e-010	6.342e-010	-9.112	-9.198	-0.086
Cl	7.531e-003				
Cl-	7.531e-003	6.109e-003	-2.123	-2.214	-0.091
MnCl+	1.711e-007	1.403e-007	-6.767	-6.853	-0.086
FeCl+	1.371e-008	1.124e-008	-7.863	-7.949	-0.086
ZnCl+	4.842e-009	3.970e-009	-8.315	-8.401	-0.086
MnCl2	3.696e-010	3.741e-010	-9.432	-9.427	0.005
ZnCl2	2.462e-011	2.491e-011	-10.609	-10.604	0.005
MnCl3-	7.676e-013	6.294e-013	-12.115	-12.201	-0.086
ZnCl3-	2.024e-013	1.659e-013	-12.694	-12.780	-0.086
ZnCl4-2	1.082e-015	4.892e-016	-14.966	-15.311	-0.345
FeCl+2	7.610e-023	3.440e-023	-22.119	-22.464	-0.345
FeCl2+	1.332e-024	1.092e-024	-23.876	-23.962	-0.086
FeCl3	6.590e-028	6.670e-028	-27.181	-27.176	0.005
Fe (2)	7.162e-006				
FeHCO3+	4.114e-006	3.373e-006	-5.386	-5.472	-0.086
Fe+2	2.781e-006	1.333e-006	-5.556	-5.875	-0.319
FeSO4	9.790e-008	9.909e-008	-7.009	-7.004	0.005

FeCO ₃	9.125e-008	9.236e-008	-7.040	-7.035	0.005
FeS	5.461e-008	5.528e-008	-7.263	-7.257	0.005
FeCl ₁ +	1.371e-008	1.124e-008	-7.863	-7.949	-0.086
Fe (HS) 2	6.997e-009	7.082e-009	-8.155	-8.150	0.005
Fe (CO ₃) (OH) -	1.178e-009	9.656e-010	-8.929	-9.015	-0.086
FeOH+	9.671e-010	7.930e-010	-9.015	-9.101	-0.086
Fe (CO ₃) 2-2	6.933e-010	3.134e-010	-9.159	-9.504	-0.345
Fe (HS) 3-	2.296e-012	1.883e-012	-11.639	-11.725	-0.086
FeHSO ₄ +	2.913e-013	2.388e-013	-12.536	-12.622	-0.086
Fe (OH) 2	2.335e-014	2.364e-014	-13.632	-13.626	0.005
Fe (3)	3.167e-015				
Fe (OH) 2+	2.573e-015	2.110e-015	-14.590	-14.676	-0.086
Fe (OH) 3	5.860e-016	5.931e-016	-15.232	-15.227	0.005
FeOH+2	6.287e-018	2.841e-018	-17.202	-17.546	-0.345
Fe (OH) 4-	1.463e-018	1.200e-018	-17.835	-17.921	-0.086
FeSO ₄ +	1.190e-021	9.760e-022	-20.924	-21.011	-0.086
Fe+3	9.081e-022	2.169e-022	-21.042	-21.664	-0.622
FeCl ₁ +2	7.610e-023	3.440e-023	-22.119	-22.464	-0.345
Fe (SO ₄) 2-	1.166e-023	9.559e-024	-22.933	-23.020	-0.086
FeCl ₁₂ +	1.332e-024	1.092e-024	-23.876	-23.962	-0.086
FeHSO ₄ +2	2.159e-027	9.760e-028	-26.666	-27.011	-0.345
FeCl ₁₃	6.590e-028	6.670e-028	-27.181	-27.176	0.005
Fe ₂ (OH) 2+4	6.344e-033	2.647e-034	-32.198	-33.577	-1.380
Fe ₃ (OH) 4+5	0.000e+000	0.000e+000	-43.586	-45.742	-2.156
H (0)	4.134e-011				
H ₂	2.067e-011	2.092e-011	-10.685	-10.679	0.005
K	6.624e-004				
K+	6.604e-004	5.357e-004	-3.180	-3.271	-0.091
KSO ₄ -	1.927e-006	1.580e-006	-5.715	-5.801	-0.086
KOH	4.932e-012	4.992e-012	-11.307	-11.302	0.005
Mg	4.689e-003				
Mg+2	3.853e-003	1.856e-003	-2.414	-2.731	-0.317
MgHCO ₃ +	6.578e-004	5.393e-004	-3.182	-3.268	-0.086
MgSO ₄	1.734e-004	1.755e-004	-3.761	-3.756	0.005
MgCO ₃	4.701e-006	4.758e-006	-5.328	-5.323	0.005
MgOH+	6.192e-009	5.077e-009	-8.208	-8.294	-0.086
Mn (2)	2.912e-005				
MnHCO ₃ +	1.550e-005	1.271e-005	-4.810	-4.896	-0.086
Mn+2	1.176e-005	5.637e-006	-4.930	-5.249	-0.319
MnCO ₃	1.278e-006	1.293e-006	-5.894	-5.888	0.005
MnSO ₄	4.124e-007	4.174e-007	-6.385	-6.379	0.005
MnCl ₁ +	1.711e-007	1.403e-007	-6.767	-6.853	-0.086
MnCl ₁₂	3.696e-010	3.741e-010	-9.432	-9.427	0.005
MnOH+	3.218e-010	2.638e-010	-9.492	-9.579	-0.086
MnCl ₁₃ -	7.676e-013	6.294e-013	-12.115	-12.201	-0.086
Mn (3)	1.146e-033				
Mn+3	1.146e-033	1.920e-034	-32.941	-33.717	-0.776
Na	1.453e-002				
Na+	1.433e-002	1.178e-002	-1.844	-1.929	-0.085
NaHCO ₃	1.656e-004	1.676e-004	-3.781	-3.776	0.005
NaSO ₄ -	3.186e-005	2.613e-005	-4.497	-4.583	-0.086
NaCO ₃ -	6.072e-007	4.979e-007	-6.217	-6.303	-0.086
NaOH	2.067e-010	2.092e-010	-9.685	-9.680	0.005
O (0)	0.000e+000				

O2	0.000e+000	0.000e+000	-72.569	-72.564	0.005
S (-2)	1.216e-005				
H2S	9.079e-006	9.190e-006	-5.042	-5.037	0.005
HS-	3.015e-006	2.441e-006	-5.521	-5.612	-0.092
FeS	5.461e-008	5.528e-008	-7.263	-7.257	0.005
Fe (HS) 2	6.997e-009	7.082e-009	-8.155	-8.150	0.005
Fe (HS) 3-	2.296e-012	1.883e-012	-11.639	-11.725	-0.086
S-2	1.242e-012	5.722e-013	-11.906	-12.242	-0.337
S (6)	1.509e-003				
SO4-2	9.951e-004	4.561e-004	-3.002	-3.341	-0.339
CaSO4	3.044e-004	3.081e-004	-3.516	-3.511	0.005
MgSO4	1.734e-004	1.755e-004	-3.761	-3.756	0.005
NaSO4-	3.186e-005	2.613e-005	-4.497	-4.583	-0.086
KSO4-	1.927e-006	1.580e-006	-5.715	-5.801	-0.086
SrSO4	1.736e-006	1.757e-006	-5.761	-5.755	0.005
BaSO4	4.462e-007	4.516e-007	-6.350	-6.345	0.005
MnSO4	4.124e-007	4.174e-007	-6.385	-6.379	0.005
FeSO4	9.790e-008	9.909e-008	-7.009	-7.004	0.005
ZnSO4	3.035e-008	3.072e-008	-7.518	-7.513	0.005
HSO4-	1.817e-008	1.490e-008	-7.741	-7.827	-0.086
CaHSO4+	7.735e-010	6.342e-010	-9.112	-9.198	-0.086
Zn (SO4) 2-2	2.614e-010	1.182e-010	-9.583	-9.928	-0.345
FeHSO4+	2.913e-013	2.388e-013	-12.536	-12.622	-0.086
FeSO4+	1.190e-021	9.760e-022	-20.924	-21.011	-0.086
Fe (SO4) 2-	1.166e-023	9.559e-024	-22.933	-23.020	-0.086
FeHSO4+2	2.159e-027	9.760e-028	-26.666	-27.011	-0.345
Si	2.963e-004				
H4SiO4	2.961e-004	2.997e-004	-3.529	-3.523	0.005
H3SiO4-	1.226e-007	1.005e-007	-6.912	-6.998	-0.086
H2SiO4-2	2.972e-014	1.343e-014	-13.527	-13.872	-0.345
Sr	5.433e-005				
Sr+2	4.423e-005	2.090e-005	-4.354	-4.680	-0.326
SrHCO3+	8.325e-006	6.886e-006	-5.080	-5.162	-0.082
SrSO4	1.736e-006	1.757e-006	-5.761	-5.755	0.005
SrCO3	3.313e-008	3.353e-008	-7.480	-7.475	0.005
SrOH+	3.496e-012	2.880e-012	-11.456	-11.541	-0.084
Zn	2.035e-006				
ZnHCO3+	1.158e-006	9.495e-007	-5.936	-6.023	-0.086
Zn+2	6.472e-007	2.981e-007	-6.189	-6.526	-0.337
ZnCO3	1.697e-007	1.717e-007	-6.770	-6.765	0.005
ZnSO4	3.035e-008	3.072e-008	-7.518	-7.513	0.005
Zn (CO3) 2-2	2.346e-008	1.060e-008	-7.630	-7.975	-0.345
ZnCl+	4.842e-009	3.970e-009	-8.315	-8.401	-0.086
ZnOH+	7.457e-010	6.114e-010	-9.127	-9.214	-0.086
Zn (SO4) 2-2	2.614e-010	1.182e-010	-9.583	-9.928	-0.345
Zn (OH) 2	2.678e-011	2.710e-011	-10.572	-10.567	0.005
ZnCl2	2.462e-011	2.491e-011	-10.609	-10.604	0.005
ZnCl3-	2.024e-013	1.659e-013	-12.694	-12.780	-0.086
ZnCl4-2	1.082e-015	4.892e-016	-14.966	-15.311	-0.345
Zn (OH) 3-	2.809e-016	2.303e-016	-15.551	-15.638	-0.086
Zn (OH) 4-2	2.170e-022	9.809e-023	-21.663	-22.008	-0.345

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH)5]	-5.35	17.74	23.09	Fe2(OH)5
[Fe3(OH)7]	-0.26	24.73	24.99	Fe3(OH)7
[Fe3(OH)8]	-13.62	28.50	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-27.30	31.05	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-27.13	33.25	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-20.49	23.07	43.56	Fe4(OH)8(Cl)1
Anhydrite	-1.45	-5.79	-4.34	CaSO4
Aragonite	0.32	-7.99	-8.31	CaCO3
Barite	1.00	-9.05	-10.05	BaSO4
Brucite	-6.66	10.13	16.79	Mg(OH)2
Calcite	0.46	-7.99	-8.45	CaCO3
Celestite	-1.40	-8.02	-6.62	SrSO4
Chalcedony	0.08	-3.52	-3.61	SiO2
Chrysotile	-9.45	23.34	32.79	Mg3Si2O5(OH)4
CO2(g)	-0.24	-1.65	-1.41	CO2
Dolomite	0.72	-16.26	-16.98	CaMg(CO3)2
Epsomite	-3.90	-6.08	-2.17	MgSO4:7H2O
Fe(OH)2(1)	-5.96	6.98	12.94	Fe(OH)2
Fe(OH)2(2)	-6.91	6.98	13.89	Fe(OH)2
Fe(OH)3(a)	-7.27	-2.38	4.89	Fe(OH)3
FeO	-6.61	6.98	13.59	FeO
FeS(am)	-1.20	-5.06	-3.86	FeS
FeS(ppt)	-1.14	-5.06	-3.92	FeS
Goethite	-1.55	-2.38	-0.83	FeOOH
Greigite	-7.27	-45.93	-38.66	Fe3S4
Gypsum	-1.21	-5.79	-4.58	CaSO4:2H2O
H2(g)	-7.55	-10.68	-3.13	H2
H2O(g)	-1.63	-0.00	1.63	H2O
H2S(g)	-4.09	-5.04	-0.94	H2S
Halite	-5.71	-4.14	1.57	NaCl
Hausmannite	-31.83	30.38	62.21	Mn3O4
Hematite	-1.10	-4.75	-3.65	Fe2O3
Jarosite-H3O	-28.07	-39.53	-11.46	H3OFe3(SO4)2(OH)6
Jarosite-K	-25.49	-36.37	-10.87	KFe3(SO4)2(OH)6
Lepidocrocite	-5.94	10.76	16.70	FeOOH
Lime	-12.40	10.41	22.81	Ca(OH)2
Mackinawite	-0.46	-5.06	-4.60	FeS
Mackinawite(2)	-1.55	1.95	3.50	FeS
Magnetite	-17.30	28.50	45.80	Fe3O4
Manganite	-13.96	11.38	25.34	MnOOH
Marcasite	8.33	-9.55	-17.88	FeS2
Melanterite	-6.95	-9.22	-2.27	FeSO4:7H2O
Nesquehonite	-2.72	-8.27	-5.55	MgCO3:3H2O
O2(g)	-69.63	-72.56	-2.94	O2
Pyrite	9.06	-9.55	-18.61	FeS2
Pyrochroite	-7.59	7.61	15.20	Mn(OH)2
Pyrolusite	-26.98	15.16	42.14	MnO2
Quartz	0.53	-3.52	-4.05	SiO2
Rhodochrosite	0.32	-10.79	-11.11	MnCO3
Schwertmannite(1)	-58.67	-48.17	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-53.20	-35.20	18.00	Fe8O8(OH)6SO4
Sepiolite	-6.20	9.69	15.89	Mg2Si3O7.5OH:3H2O

Sepiolite(d)	-8.97	9.69	18.66	Mg ₂ Si ₃ O ₇ .5OH:3H ₂ O
Siderite	-0.55	-11.41	-10.86	FeCO ₃
SiO ₂ (a)	-0.77	-3.52	-2.75	SiO ₂
Smithsonite	-2.12	-12.07	-9.95	ZnCO ₃
Sphalerite	6.01	-5.71	-11.71	ZnS
Strontianite	-0.95	-10.22	-9.27	SrCO ₃
Sulfur	-2.48	2.51	4.99	S
Talc	-5.65	16.30	21.94	Mg ₃ Si ₄ O ₁₀ (OH) ₂
Troilite	1.09	-5.06	-6.15	FeS
Willemite	-6.58	9.15	15.72	Zn ₂ SiO ₄
Witherite	-2.67	-11.24	-8.57	BaCO ₃
Zn(OH) ₂ (e)	-5.17	6.33	11.50	Zn(OH) ₂

End of simulation.

Reading input data for simulation 9.

SOLUTION 1 MP2 9-6-2007

temp	19.4
pH	6.48
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Fe	0.2
S(6)	1220 as SO ₄
S(-2)	0.59
Cl	283
Br	0.29
Alkalinity	2200 as HCO ₃
Ba	0.221
Ca	779
Mg	141
Na	418
K	58.1
Mn	0.94
Si	19.0
Sr	6.06
Zn	0.076
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. MP2 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
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Alkalinity	3.605e-002	3.605e-002
Ba	1.609e-006	1.609e-006
Br	3.629e-006	3.629e-006
Ca	1.944e-002	1.944e-002
Cl	7.982e-003	7.982e-003
Fe	3.581e-006	3.581e-006
K	1.486e-003	1.486e-003
Mg	5.800e-003	5.800e-003
Mn	1.711e-005	1.711e-005
Na	1.818e-002	1.818e-002
S(-2)	1.840e-005	1.840e-005
S(6)	1.270e-002	1.270e-002
Si	3.162e-004	3.162e-004
Sr	6.916e-005	6.916e-005
Zn	1.163e-006	1.163e-006

-----Description of solution-----

pH	=	6.480
pe	=	4.000
Activity of water	=	0.998
Ionic strength	=	8.337e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	5.685e-002
Total CO2 (mol/kg)	=	5.685e-002
Temperature (deg C)	=	19.400
Electrical balance (eq)	=	8.845e-004
Percent error, 100*(Cat- An)/(Cat+ An)	=	0.77
Iterations	=	10
Total H	=	1.110497e+002
Total O	=	5.570799e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.6146	-0.1518

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.969e-007	3.311e-007	-6.401	-6.480	-0.079
OH-	2.510e-008	1.950e-008	-7.600	-7.710	-0.109
H2O	5.551e+001	9.980e-001	1.744	-0.001	0.000
Ba	1.609e-006				
Ba+2	9.287e-007	3.734e-007	-6.032	-6.428	-0.396
BaSO4	5.803e-007	5.916e-007	-6.236	-6.228	0.008
BaHCO3+	9.959e-008	7.903e-008	-7.002	-7.102	-0.100
BaCO3	5.586e-010	5.695e-010	-9.253	-9.245	0.008
BaOH+	4.805e-014	3.813e-014	-13.318	-13.419	-0.100
Br	3.629e-006				

Br-	3.629e-006	2.795e-006	-5.440	-5.554	-0.114
C (4)	5.685e-002				
HCO3-	3.289e-002	2.634e-002	-1.483	-1.579	-0.096
CO2	2.085e-002	2.125e-002	-1.681	-1.673	0.008
CaHCO3+	2.190e-003	1.754e-003	-2.660	-2.756	-0.096
MgHCO3+	6.605e-004	5.241e-004	-3.180	-3.281	-0.100
NaHCO3	2.046e-004	2.086e-004	-3.689	-3.681	0.008
CaCO3	2.829e-005	2.884e-005	-4.548	-4.540	0.008
SrHCO3+	8.507e-006	6.813e-006	-5.070	-5.167	-0.096
MnHCO3+	8.302e-006	6.588e-006	-5.081	-5.181	-0.100
CO3-2	8.032e-006	3.304e-006	-5.095	-5.481	-0.386
MgCO3	4.932e-006	5.027e-006	-5.307	-5.299	0.008
FeHCO3+	1.872e-006	1.486e-006	-5.728	-5.828	-0.100
NaCO3-	8.186e-007	6.496e-007	-6.087	-6.187	-0.100
MnCO3	7.225e-007	7.365e-007	-6.141	-6.133	0.008
ZnHCO3+	5.929e-007	4.705e-007	-6.227	-6.327	-0.100
BaHCO3+	9.959e-008	7.903e-008	-7.002	-7.102	-0.100
ZnCO3	9.176e-008	9.354e-008	-7.037	-7.029	0.008
FeCO3	4.386e-008	4.471e-008	-7.358	-7.350	0.008
SrCO3	3.592e-008	3.661e-008	-7.445	-7.436	0.008
Zn (CO3) 2-2	1.666e-008	6.607e-009	-7.778	-8.180	-0.402
Fe (CO3) (OH) -	6.606e-010	5.242e-010	-9.180	-9.280	-0.100
BaCO3	5.586e-010	5.695e-010	-9.253	-9.245	0.008
Fe (CO3) 2-2	4.377e-010	1.735e-010	-9.359	-9.761	-0.402
Ca	1.944e-002				
Ca+2	1.385e-002	5.746e-003	-1.859	-2.241	-0.382
CaSO4	3.371e-003	3.436e-003	-2.472	-2.464	0.008
CaHCO3+	2.190e-003	1.754e-003	-2.660	-2.756	-0.096
CaCO3	2.829e-005	2.884e-005	-4.548	-4.540	0.008
CaHSO4+	7.864e-009	6.240e-009	-8.104	-8.205	-0.100
CaOH+	3.622e-009	2.874e-009	-8.441	-8.541	-0.100
Cl	7.982e-003				
Cl-	7.982e-003	6.222e-003	-2.098	-2.206	-0.108
MnCl+	8.964e-008	7.113e-008	-7.047	-7.148	-0.100
FeCl+	6.105e-009	4.845e-009	-8.214	-8.315	-0.100
ZnCl+	2.328e-009	1.848e-009	-8.633	-8.733	-0.100
MnCl2	1.895e-010	1.932e-010	-9.722	-9.714	0.008
ZnCl2	1.154e-011	1.176e-011	-10.938	-10.929	0.008
MnCl3-	4.172e-013	3.310e-013	-12.380	-12.480	-0.100
ZnCl3-	1.000e-013	7.935e-014	-13.000	-13.100	-0.100
ZnCl4-2	5.964e-016	2.365e-016	-15.224	-15.626	-0.402
FeCl+2	3.785e-023	1.501e-023	-22.422	-22.824	-0.402
FeCl2+	6.298e-025	4.998e-025	-24.201	-24.301	-0.100
FeCl3	3.050e-028	3.110e-028	-27.516	-27.507	0.008
Fe (2)	3.581e-006				
FeHCO3+	1.872e-006	1.486e-006	-5.728	-5.828	-0.100
Fe+2	1.328e-006	5.641e-007	-5.877	-6.249	-0.372
FeSO4	2.803e-007	2.857e-007	-6.552	-6.544	0.008
FeCO3	4.386e-008	4.471e-008	-7.358	-7.350	0.008
FeS	4.136e-008	4.216e-008	-7.383	-7.375	0.008
Fe (HS) 2	7.587e-009	7.734e-009	-8.120	-8.112	0.008
FeCl+	6.105e-009	4.845e-009	-8.214	-8.315	-0.100
Fe (CO3) (OH) -	6.606e-010	5.242e-010	-9.180	-9.280	-0.100
FeOH+	4.423e-010	3.510e-010	-9.354	-9.455	-0.100

Fe (CO ₃) ²⁻²	4.377e-010	1.735e-010	-9.359	-9.761	-0.402
Fe (HS) ³⁻	4.163e-012	3.303e-012	-11.381	-11.481	-0.100
FeHSO ₄ ⁺	7.720e-013	6.126e-013	-12.112	-12.213	-0.100
Fe (OH) ²	1.234e-014	1.258e-014	-13.909	-13.900	0.008
Fe (3)	1.670e-015				
Fe (OH) ²⁺	1.348e-015	1.070e-015	-14.870	-14.971	-0.100
Fe (OH) ³	3.178e-016	3.239e-016	-15.498	-15.490	0.008
FeOH ²	3.357e-018	1.331e-018	-17.474	-17.876	-0.402
Fe (OH) ⁴⁻	8.922e-019	7.080e-019	-18.050	-18.150	-0.100
FeSO ₄ ⁺	3.685e-021	2.924e-021	-20.434	-20.534	-0.100
Fe ³	4.892e-022	9.572e-023	-21.311	-22.019	-0.708
Fe (SO ₄) ²⁻	2.493e-022	1.978e-022	-21.603	-21.704	-0.100
FeCl ¹⁺²	3.785e-023	1.501e-023	-22.422	-22.824	-0.402
FeCl ₂ ⁺	6.298e-025	4.998e-025	-24.201	-24.301	-0.100
FeHSO ₄ ²	6.585e-027	2.611e-027	-26.181	-26.583	-0.402
FeCl ₃	3.050e-028	3.110e-028	-27.516	-27.507	0.008
Fe ₂ (OH) ²⁺⁴	2.443e-033	6.038e-035	-32.612	-34.219	-1.607
Fe ₃ (OH) ⁴⁺⁵	0.000e+000	0.000e+000	-44.130	-46.641	-2.511
H (0)	2.732e-011				
H ₂	1.366e-011	1.392e-011	-10.865	-10.856	0.008
K	1.486e-003				
K ⁺	1.457e-003	1.136e-003	-2.837	-2.945	-0.108
KSO ₄ ⁻	2.878e-005	2.284e-005	-4.541	-4.641	-0.100
KOH	1.164e-011	1.187e-011	-10.934	-10.926	0.008
Mg	5.800e-003				
Mg ²	4.043e-003	1.738e-003	-2.393	-2.760	-0.367
MgSO ₄	1.091e-003	1.112e-003	-2.962	-2.954	0.008
MgHCO ₃ ⁺	6.605e-004	5.241e-004	-3.180	-3.281	-0.100
MgCO ₃	4.932e-006	5.027e-006	-5.307	-5.299	0.008
MgOH ⁺	6.177e-009	4.902e-009	-8.209	-8.310	-0.100
Mn (2)	1.711e-005				
MnHCO ₃ ⁺	8.302e-006	6.588e-006	-5.081	-5.181	-0.100
Mn ²	6.607e-006	2.806e-006	-5.180	-5.552	-0.372
MnSO ₄	1.388e-006	1.415e-006	-5.858	-5.849	0.008
MnCO ₃	7.225e-007	7.365e-007	-6.141	-6.133	0.008
MnCl ¹⁺	8.964e-008	7.113e-008	-7.047	-7.148	-0.100
MnCl ₂	1.895e-010	1.932e-010	-9.722	-9.714	0.008
MnOH ⁺	1.721e-010	1.365e-010	-9.764	-9.865	-0.100
MnCl ₃ ⁻	4.172e-013	3.310e-013	-12.380	-12.480	-0.100
Mn (3)	7.337e-034				
Mn ³	7.337e-034	9.154e-035	-33.134	-34.038	-0.904
Na	1.818e-002				
Na ⁺	1.771e-002	1.408e-002	-1.752	-1.851	-0.099
NaSO ₄ ⁻	2.712e-004	2.152e-004	-3.567	-3.667	-0.100
NaHCO ₃	2.046e-004	2.086e-004	-3.689	-3.681	0.008
NaCO ₃ ⁻	8.186e-007	6.496e-007	-6.087	-6.187	-0.100
NaOH	2.751e-010	2.804e-010	-9.561	-9.552	0.008
O (0)	0.000e+000				
O ₂	0.000e+000	0.000e+000	-72.519	-72.511	0.008
S (-2)	1.840e-005				
H ₂ S	1.330e-005	1.356e-005	-4.876	-4.868	0.008
HS ⁻	5.047e-006	3.922e-006	-5.297	-5.406	-0.109
FeS	4.136e-008	4.216e-008	-7.383	-7.375	0.008
Fe (HS) ²	7.587e-009	7.734e-009	-8.120	-8.112	0.008

Fe (HS) 3-	4.163e-012	3.303e-012	-11.381	-11.481	-0.100
S-2	2.407e-012	9.677e-013	-11.619	-12.014	-0.396
S (6)	1.270e-002				
SO4-2	7.924e-003	3.161e-003	-2.101	-2.500	-0.399
CaSO4	3.371e-003	3.436e-003	-2.472	-2.464	0.008
MgSO4	1.091e-003	1.112e-003	-2.962	-2.954	0.008
NaSO4-	2.712e-004	2.152e-004	-3.567	-3.667	-0.100
KSO4-	2.878e-005	2.284e-005	-4.541	-4.641	-0.100
SrSO4	1.158e-005	1.181e-005	-4.936	-4.928	0.008
MnSO4	1.388e-006	1.415e-006	-5.858	-5.849	0.008
BaSO4	5.803e-007	5.916e-007	-6.236	-6.228	0.008
FeSO4	2.803e-007	2.857e-007	-6.552	-6.544	0.008
HSO4-	1.138e-007	9.033e-008	-6.944	-7.044	-0.100
ZnSO4	9.873e-008	1.006e-007	-7.006	-6.997	0.008
CaHSO4+	7.864e-009	6.240e-009	-8.104	-8.205	-0.100
Zn (SO4) 2-2	6.815e-009	2.702e-009	-8.167	-8.568	-0.402
FeHSO4+	7.720e-013	6.126e-013	-12.112	-12.213	-0.100
FeSO4+	3.685e-021	2.924e-021	-20.434	-20.534	-0.100
Fe (SO4) 2-	2.493e-022	1.978e-022	-21.603	-21.704	-0.100
FeHSO4+2	6.585e-027	2.611e-027	-26.181	-26.583	-0.402
Si	3.162e-004				
H4SiO4	3.161e-004	3.222e-004	-3.500	-3.492	0.008
H3SiO4-	1.477e-007	1.172e-007	-6.831	-6.931	-0.100
H2SiO4-2	4.166e-014	1.652e-014	-13.380	-13.782	-0.402
Sr	6.916e-005				
Sr+2	4.904e-005	2.048e-005	-4.309	-4.689	-0.379
SrSO4	1.158e-005	1.181e-005	-4.936	-4.928	0.008
SrHCO3+	8.507e-006	6.813e-006	-5.070	-5.167	-0.096
SrCO3	3.592e-008	3.661e-008	-7.445	-7.436	0.008
SrOH+	3.976e-012	3.166e-012	-11.401	-11.499	-0.099
Zn	1.163e-006				
ZnHCO3+	5.929e-007	4.705e-007	-6.227	-6.327	-0.100
Zn+2	3.530e-007	1.419e-007	-6.452	-6.848	-0.396
ZnSO4	9.873e-008	1.006e-007	-7.006	-6.997	0.008
ZnCO3	9.176e-008	9.354e-008	-7.037	-7.029	0.008
Zn (CO3) 2-2	1.666e-008	6.607e-009	-7.778	-8.180	-0.402
Zn (SO4) 2-2	6.815e-009	2.702e-009	-8.167	-8.568	-0.402
ZnCl+	2.328e-009	1.848e-009	-8.633	-8.733	-0.100
ZnOH+	3.833e-010	3.042e-010	-9.416	-9.517	-0.100
Zn (OH) 2	1.592e-011	1.623e-011	-10.798	-10.790	0.008
ZnCl2	1.154e-011	1.176e-011	-10.938	-10.929	0.008
ZnCl3-	1.000e-013	7.935e-014	-13.000	-13.100	-0.100
ZnCl4-2	5.964e-016	2.365e-016	-15.224	-15.626	-0.402
Zn (OH) 3-	1.949e-016	1.547e-016	-15.710	-15.811	-0.100
Zn (OH) 4-2	1.864e-022	7.389e-023	-21.730	-22.131	-0.402

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-5.81	17.28	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	-1.00	23.99	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-14.26	27.86	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-28.80	29.55	58.35	Fe6 (OH) 12 (CO3) 1

[Fe6(OH)12][SO4]	-27.85	32.53	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-21.54	22.02	43.56	Fe4(OH)8(Cl)1
Anhydrite	-0.40	-4.74	-4.34	CaSO4
Aragonite	0.58	-7.72	-8.30	CaCO3
Barite	1.14	-8.93	-10.06	BaSO4
Brucite	-6.59	10.20	16.79	Mg(OH)2
Calcite	0.73	-7.72	-8.45	CaCO3
Celestite	-0.57	-7.19	-6.62	SrSO4
Chalcedony	0.13	-3.49	-3.62	SiO2
Chrysotile	-9.29	23.62	32.91	Mg3Si2O5(OH)4
CO2(g)	-0.27	-1.67	-1.40	CO2
Dolomite	1.00	-15.96	-16.96	CaMg(CO3)2
Epsomite	-3.09	-5.27	-2.18	MgSO4·7H2O
Fe(OH)2(1)	-6.23	6.71	12.94	Fe(OH)2
Fe(OH)2(2)	-7.18	6.71	13.89	Fe(OH)2
Fe(OH)3(a)	-7.47	-2.58	4.89	Fe(OH)3
FeO	-6.88	6.71	13.59	FeO
FeS(am)	-1.33	-5.18	-3.85	FeS
FeS(ppt)	-1.26	-5.18	-3.92	FeS
Goethite	-1.78	-2.58	-0.80	FeOOH
Greigite	-7.35	-45.99	-38.64	Fe3S4
Gypsum	-0.16	-4.74	-4.58	CaSO4·2H2O
H2(g)	-7.73	-10.86	-3.13	H2
H2O(g)	-1.66	-0.00	1.66	H2O
H2S(g)	-3.94	-4.87	-0.93	H2S
Halite	-5.63	-4.06	1.57	NaCl
Hausmannite	-32.49	29.95	62.44	Mn3O4
Hematite	-1.59	-5.16	-3.58	Fe2O3
Jarosite-H3O	-27.33	-38.66	-11.34	H3OFe3(SO4)2(OH)6
Jarosite-K	-24.28	-35.13	-10.85	KFe3(SO4)2(OH)6
Lepidocrocite	-6.12	10.58	16.70	FeOOH
Lime	-12.09	10.72	22.81	Ca(OH)2
Mackinawite	-0.58	-5.18	-4.59	FeS
Mackinawite(2)	-1.66	1.84	3.50	FeS
Magnetite	-17.94	27.86	45.80	Fe3O4
Manganite	-14.07	11.27	25.34	MnOOH
Marcasite	8.58	-9.33	-17.91	FeS2
Melanterite	-6.48	-8.75	-2.28	FeSO4·7H2O
Nesquehonite	-2.70	-8.24	-5.54	MgCO3·3H2O
O2(g)	-69.58	-72.51	-2.93	O2
Pyrite	9.31	-9.33	-18.64	FeS2
Pyrochroite	-7.79	7.41	15.20	Mn(OH)2
Pyrolusite	-27.16	15.14	42.29	MnO2
Quartz	0.57	-3.49	-4.06	SiO2
Rhodochrosite	0.08	-11.03	-11.11	MnCO3
Schwertmannite(1)	-58.98	-48.48	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-54.10	-36.10	18.00	Fe8O8(OH)6SO4
Sepiolite	-5.99	9.92	15.91	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-8.74	9.92	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-0.87	-11.73	-10.86	FeCO3
SiO2(a)	-0.73	-3.49	-2.76	SiO2
Smithsonite	-2.39	-12.33	-9.94	ZnCO3
Sphalerite	5.96	-5.77	-11.73	ZnS
Strontianite	-0.90	-10.17	-9.27	SrCO3

Sulfur	-2.15	2.86	5.02	S
Talc	-5.41	16.64	22.05	Mg ₃ Si ₄ O ₁₀ (OH) ₂
Troilite	0.97	-5.18	-6.15	FeS
Willemite	-7.07	8.73	15.80	Zn ₂ SiO ₄
Witherite	-3.33	-11.91	-8.58	BaCO ₃
Zn(OH) ₂ (e)	-5.39	6.11	11.50	Zn(OH) ₂

End of simulation.

Reading input data for simulation 10.

SOLUTION 1 MP3 9-6-2007

temp	20.4
pH	6.44
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Fe	2.95
S(6)	1480 as SO ₄
S(-2)	0.02
Cl	267
Br	1.6
Alkalinity	1100 as HCO ₃
Ba	0.019
Ca	595
Mg	138
Na	427
K	12.3
Mn	1.13
Si	11.4
Sr	6.65
Zn	0.057
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. MP3 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.803e-002	1.803e-002
Ba	1.383e-007	1.383e-007
Br	2.002e-005	2.002e-005
Ca	1.485e-002	1.485e-002
Cl	7.531e-003	7.531e-003

Fe	5.282e-005	5.282e-005
K	3.146e-004	3.146e-004
Mg	5.676e-003	5.676e-003
Mn	2.057e-005	2.057e-005
Na	1.857e-002	1.857e-002
S(-2)	6.238e-007	6.238e-007
S(6)	1.541e-002	1.541e-002
Si	1.897e-004	1.897e-004
Sr	7.590e-005	7.590e-005
Zn	8.720e-007	8.720e-007

-----Description of solution-----

pH	=	6.440
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	7.078e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	2.955e-002
Total CO2 (mol/kg)	=	2.955e-002
Temperature (deg C)	=	20.400
Electrical balance (eq)	=	3.841e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	4.13
Iterations	=	11
Total H	=	1.110312e+002
Total O	=	5.564571e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.3856	-0.1389

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	4.319e-007	3.631e-007	-6.365	-6.440	-0.075
OH-	2.444e-008	1.928e-008	-7.612	-7.715	-0.103
H2O	5.551e+001	9.985e-001	1.744	-0.001	0.000
Ba	1.383e-007				
Ba+2	7.169e-008	3.026e-008	-7.145	-7.519	-0.375
BaSO4	6.242e-008	6.344e-008	-7.205	-7.198	0.007
BaHCO3+	4.213e-009	3.381e-009	-8.375	-8.471	-0.095
BaCO3	2.212e-011	2.248e-011	-10.655	-10.648	0.007
BaOH+	3.513e-015	2.820e-015	-14.454	-14.550	-0.095
Br	2.002e-005				
Br-	2.002e-005	1.567e-005	-4.698	-4.805	-0.107
C(4)	2.955e-002				
HCO3-	1.663e-002	1.347e-002	-1.779	-1.870	-0.091
CO2	1.154e-002	1.173e-002	-1.938	-1.931	0.007
CaHCO3+	8.858e-004	7.176e-004	-3.053	-3.144	-0.091
MgHCO3+	3.332e-004	2.675e-004	-3.477	-3.573	-0.095

NaHCO ₃	1.085e-004	1.103e-004	-3.964	-3.957	0.007
FeHCO ₃ +	1.904e-005	1.528e-005	-4.720	-4.816	-0.095
CaCO ₃	1.081e-005	1.098e-005	-4.966	-4.959	0.007
MnHCO ₃ +	6.728e-006	5.400e-006	-5.172	-5.268	-0.095
SrHCO ₃ +	5.045e-006	4.087e-006	-5.297	-5.389	-0.091
CO ₃ -2	3.661e-006	1.577e-006	-5.436	-5.802	-0.366
MgCO ₃	2.384e-006	2.423e-006	-5.623	-5.616	0.007
MnCO ₃	5.542e-007	5.633e-007	-6.256	-6.249	0.007
FeCO ₃	4.222e-007	4.292e-007	-6.374	-6.367	0.007
NaCO ₃ -	4.209e-007	3.379e-007	-6.376	-6.471	-0.095
ZnHCO ₃ +	3.151e-007	2.529e-007	-6.502	-6.597	-0.095
ZnCO ₃	4.616e-008	4.692e-008	-7.336	-7.329	0.007
SrCO ₃	2.007e-008	2.040e-008	-7.697	-7.690	0.007
Fe (CO ₃) (OH) -	5.721e-009	4.592e-009	-8.243	-8.338	-0.095
BaHCO ₃ +	4.213e-009	3.381e-009	-8.375	-8.471	-0.095
Zn (CO ₃) 2-2	3.812e-009	1.582e-009	-8.419	-8.801	-0.382
Fe (CO ₃) 2-2	1.916e-009	7.953e-010	-8.718	-9.099	-0.382
BaCO ₃	2.212e-011	2.248e-011	-10.655	-10.648	0.007
Ca	1.485e-002				
Ca+2	1.040e-002	4.510e-003	-1.983	-2.346	-0.363
CaSO ₄	3.546e-003	3.604e-003	-2.450	-2.443	0.007
CaHCO ₃ +	8.858e-004	7.176e-004	-3.053	-3.144	-0.091
CaCO ₃	1.081e-005	1.098e-005	-4.966	-4.959	0.007
CaHSO ₄ +	9.041e-009	7.257e-009	-8.044	-8.139	-0.095
CaOH+	2.565e-009	2.059e-009	-8.591	-8.686	-0.095
Cl	7.531e-003				
Cl-	7.531e-003	5.955e-003	-2.123	-2.225	-0.102
MnCl+	1.359e-007	1.091e-007	-6.867	-6.962	-0.095
FeCl+	1.162e-007	9.324e-008	-6.935	-7.030	-0.095
ZnCl+	2.423e-009	1.945e-009	-8.616	-8.711	-0.095
MnCl ₂	2.790e-010	2.835e-010	-9.554	-9.547	0.007
ZnCl ₂	1.171e-011	1.190e-011	-10.931	-10.924	0.007
MnCl ₃ -	5.794e-013	4.650e-013	-12.237	-12.333	-0.095
ZnCl ₃ -	9.633e-014	7.732e-014	-13.016	-13.112	-0.095
ZnCl ₄ -2	5.358e-016	2.224e-016	-15.271	-15.653	-0.382
FeCl+2	1.289e-021	5.351e-022	-20.890	-21.272	-0.382
FeCl ₂ +	2.056e-023	1.651e-023	-22.687	-22.782	-0.095
FeCl ₃	9.670e-027	9.829e-027	-26.015	-26.007	0.007
Fe (2)	5.282e-005				
Fe+2	2.558e-005	1.134e-005	-4.592	-4.945	-0.353
FeHCO ₃ +	1.904e-005	1.528e-005	-4.720	-4.816	-0.095
FeSO ₄	7.622e-006	7.747e-006	-5.118	-5.111	0.007
FeCO ₃	4.222e-007	4.292e-007	-6.374	-6.367	0.007
FeCl+	1.162e-007	9.324e-008	-6.935	-7.030	-0.095
FeS	2.385e-008	2.424e-008	-7.622	-7.615	0.007
FeOH+	8.669e-009	6.958e-009	-8.062	-8.158	-0.095
Fe (CO ₃) (OH) -	5.721e-009	4.592e-009	-8.243	-8.338	-0.095
Fe (CO ₃) 2-2	1.916e-009	7.953e-010	-8.718	-9.099	-0.382
Fe (HS) 2	1.505e-010	1.529e-010	-9.823	-9.816	0.007
FeHSO ₄ +	2.274e-011	1.825e-011	-10.643	-10.739	-0.095
Fe (OH) 2	2.072e-013	2.106e-013	-12.684	-12.677	0.007
Fe (HS) 3-	2.552e-015	2.048e-015	-14.593	-14.689	-0.095
Fe (3)	5.446e-014				
Fe (OH) 2+	4.423e-014	3.550e-014	-13.354	-13.450	-0.095

Fe (OH) 3	1.009e-014	1.026e-014	-13.996	-13.989	0.007
FeOH+2	1.121e-016	4.654e-017	-15.950	-16.332	-0.382
Fe (OH) 4-	2.657e-017	2.133e-017	-16.576	-16.671	-0.095
FeSO4+	1.778e-019	1.427e-019	-18.750	-18.845	-0.095
Fe+3	1.645e-020	3.451e-021	-19.784	-20.462	-0.678
Fe (SO4) 2-	1.598e-020	1.283e-020	-19.796	-19.892	-0.095
FeCl+2	1.289e-021	5.351e-022	-20.890	-21.272	-0.382
FeCl2+	2.056e-023	1.651e-023	-22.687	-22.782	-0.095
FeHSO4+2	3.360e-025	1.395e-025	-24.474	-24.856	-0.382
FeCl3	9.670e-027	9.829e-027	-26.015	-26.007	0.007
Fe2 (OH) 2+4	2.383e-030	7.071e-032	-29.623	-31.151	-1.528
Fe3 (OH) 4+5	1.967e-040	0.000e+000	-39.706	-42.093	-2.387
H (0)	1.136e-011				
H2	5.681e-012	5.774e-012	-11.246	-11.239	0.007
K	3.146e-004				
K+	3.064e-004	2.423e-004	-3.514	-3.616	-0.102
KSO4-	8.178e-006	6.564e-006	-5.087	-5.183	-0.095
KOH	2.273e-012	2.310e-012	-11.643	-11.636	0.007
Mg	5.676e-003				
Mg+2	3.863e-003	1.728e-003	-2.413	-2.763	-0.349
MgSO4	1.478e-003	1.502e-003	-2.830	-2.823	0.007
MgHCO3+	3.332e-004	2.675e-004	-3.477	-3.573	-0.095
MgCO3	2.384e-006	2.423e-006	-5.623	-5.616	0.007
MgOH+	6.082e-009	4.882e-009	-8.216	-8.311	-0.095
Mn (2)	2.057e-005				
Mn+2	1.014e-005	4.496e-006	-4.994	-5.347	-0.353
MnHCO3+	6.728e-006	5.400e-006	-5.172	-5.268	-0.095
MnSO4	3.010e-006	3.060e-006	-5.521	-5.514	0.007
MnCO3	5.542e-007	5.633e-007	-6.256	-6.249	0.007
MnCl+	1.359e-007	1.091e-007	-6.867	-6.962	-0.095
MnCl2	2.790e-010	2.835e-010	-9.554	-9.547	0.007
MnOH+	2.706e-010	2.172e-010	-9.568	-9.663	-0.095
MnCl3-	5.794e-013	4.650e-013	-12.237	-12.333	-0.095
Mn (3)	2.090e-033				
Mn+3	2.090e-033	2.890e-034	-32.680	-33.539	-0.859
Na	1.857e-002				
Na+	1.810e-002	1.456e-002	-1.742	-1.837	-0.094
NaSO4-	3.692e-004	2.964e-004	-3.433	-3.528	-0.095
NaHCO3	1.085e-004	1.103e-004	-3.964	-3.957	0.007
NaCO3-	4.209e-007	3.379e-007	-6.376	-6.471	-0.095
NaOH	2.603e-010	2.646e-010	-9.585	-9.577	0.007
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-71.419	-71.412	0.007
S (-2)	6.238e-007				
H2S	4.437e-007	4.510e-007	-6.353	-6.346	0.007
HS-	1.559e-007	1.230e-007	-6.807	-6.910	-0.103
FeS	2.385e-008	2.424e-008	-7.622	-7.615	0.007
Fe (HS) 2	1.505e-010	1.529e-010	-9.823	-9.816	0.007
S-2	7.039e-014	2.971e-014	-13.152	-13.527	-0.375
Fe (HS) 3-	2.552e-015	2.048e-015	-14.593	-14.689	-0.095
S (6)	1.541e-002				
SO4-2	9.977e-003	4.183e-003	-2.001	-2.378	-0.377
CaSO4	3.546e-003	3.604e-003	-2.450	-2.443	0.007
MgSO4	1.478e-003	1.502e-003	-2.830	-2.823	0.007

NaSO4-	3.692e-004	2.964e-004	-3.433	-3.528	-0.095
SrSO4	1.763e-005	1.792e-005	-4.754	-4.747	0.007
KSO4-	8.178e-006	6.564e-006	-5.087	-5.183	-0.095
FeSO4	7.622e-006	7.747e-006	-5.118	-5.111	0.007
MnSO4	3.010e-006	3.060e-006	-5.521	-5.514	0.007
HSO4-	1.667e-007	1.338e-007	-6.778	-6.873	-0.095
ZnSO4	1.388e-007	1.411e-007	-6.858	-6.851	0.007
BaSO4	6.242e-008	6.344e-008	-7.205	-7.198	0.007
Zn (SO4) 2-2	1.198e-008	4.972e-009	-7.922	-8.303	-0.382
CaHSO4+	9.041e-009	7.257e-009	-8.044	-8.139	-0.095
FeHSO4+	2.274e-011	1.825e-011	-10.643	-10.739	-0.095
FeSO4+	1.778e-019	1.427e-019	-18.750	-18.845	-0.095
Fe (SO4) 2-	1.598e-020	1.283e-020	-19.796	-19.892	-0.095
FeHSO4+2	3.360e-025	1.395e-025	-24.474	-24.856	-0.382
Si	1.897e-004				
H4SiO4	1.897e-004	1.928e-004	-3.722	-3.715	0.007
H3SiO4-	8.271e-008	6.639e-008	-7.082	-7.178	-0.095
H2SiO4-2	2.203e-014	9.142e-015	-13.657	-14.039	-0.382
Sr	7.590e-005				
Sr+2	5.320e-005	2.321e-005	-4.274	-4.634	-0.360
SrSO4	1.763e-005	1.792e-005	-4.754	-4.747	0.007
SrHCO3+	5.045e-006	4.087e-006	-5.297	-5.389	-0.091
SrCO3	2.007e-008	2.040e-008	-7.697	-7.690	0.007
SrOH+	4.062e-012	3.274e-012	-11.391	-11.485	-0.094
Zn	8.720e-007				
Zn+2	3.533e-007	1.491e-007	-6.452	-6.827	-0.375
ZnHCO3+	3.151e-007	2.529e-007	-6.502	-6.597	-0.095
ZnSO4	1.388e-007	1.411e-007	-6.858	-6.851	0.007
ZnCO3	4.616e-008	4.692e-008	-7.336	-7.329	0.007
Zn (SO4) 2-2	1.198e-008	4.972e-009	-7.922	-8.303	-0.382
Zn (CO3) 2-2	3.812e-009	1.582e-009	-8.419	-8.801	-0.382
ZnCl+	2.423e-009	1.945e-009	-8.616	-8.711	-0.095
ZnOH+	3.930e-010	3.155e-010	-9.406	-9.501	-0.095
Zn (OH) 2	1.397e-011	1.420e-011	-10.855	-10.848	0.007
ZnCl2	1.171e-011	1.190e-011	-10.931	-10.924	0.007
ZnCl3-	9.633e-014	7.732e-014	-13.016	-13.112	-0.095
ZnCl4-2	5.358e-016	2.224e-016	-15.271	-15.653	-0.382
Zn (OH) 3-	1.538e-016	1.235e-016	-15.813	-15.908	-0.095
Zn (OH) 4-2	1.297e-022	5.382e-023	-21.887	-22.269	-0.382

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-3.17	19.92	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	2.86	27.85	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-10.21	31.91	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-21.32	37.03	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-19.93	40.45	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-16.44	27.12	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-0.38	-4.72	-4.34	CaSO4
Aragonite	0.16	-8.15	-8.31	CaCO3
Barite	0.15	-9.90	-10.05	BaSO4
Brucite	-6.68	10.12	16.79	Mg (OH) 2

Calcite	0.31	-8.15	-8.46	CaCO ₃
Celestite	-0.39	-7.01	-6.62	SrSO ₄
Chalcedony	-0.11	-3.71	-3.61	SiO ₂
Chrysotile	-9.86	22.92	32.78	Mg ₃ Si ₂ O ₅ (OH) ₄
CO ₂ (g)	-0.52	-1.93	-1.41	CO ₂
Dolomite	0.27	-16.71	-16.98	CaMg(CO ₃) ₂
Epsomite	-2.97	-5.15	-2.17	MgSO ₄ ·7H ₂ O
Fe(OH) ₂ (1)	-5.01	7.93	12.94	Fe(OH) ₂
Fe(OH) ₂ (2)	-5.96	7.93	13.89	Fe(OH) ₂
Fe(OH) ₃ (a)	-6.03	-1.14	4.89	Fe(OH) ₃
FeO	-5.66	7.93	13.59	FeO
FeS(am)	-1.56	-5.42	-3.86	FeS
FeS(ppt)	-1.50	-5.42	-3.92	FeS
Goethite	-0.31	-1.14	-0.83	FeOOH
Greigite	-9.08	-47.75	-38.67	Fe ₃ S ₄
Gypsum	-0.14	-4.73	-4.58	CaSO ₄ ·2H ₂ O
H ₂ (g)	-8.11	-11.24	-3.13	H ₂
H ₂ O(g)	-1.63	-0.00	1.63	H ₂ O
H ₂ S(g)	-5.40	-6.35	-0.94	H ₂ S
Halite	-5.63	-4.06	1.57	NaCl
Hausmannite	-31.48	30.70	62.19	Mn ₃ O ₄
Hematite	1.37	-2.29	-3.65	Fe ₂ O ₃
Jarosite-H ₃ O	-22.47	-33.95	-11.48	H ₃ OFe ₃ (SO ₄) ₂ (OH) ₆
Jarosite-K	-20.25	-31.12	-10.88	KFe ₃ (SO ₄) ₂ (OH) ₆
Lepidocrocite	-4.71	11.99	16.70	FeOOH
Lime	-12.28	10.53	22.81	Ca(OH) ₂
Mackinawite	-0.81	-5.42	-4.60	FeS
Mackinawite(2)	-1.91	1.59	3.50	FeS
Magnetite	-13.89	31.91	45.80	Fe ₃ O ₄
Manganite	-13.75	11.59	25.34	MnOOH
Marcasite	7.23	-10.66	-17.88	FeS ₂
Melanterite	-5.06	-7.33	-2.27	FeSO ₄ ·7H ₂ O
Nesquehonite	-3.01	-8.57	-5.55	MgCO ₃ ·3H ₂ O
O ₂ (g)	-68.47	-71.41	-2.94	O ₂
Pyrite	7.95	-10.66	-18.61	FeS ₂
Pyrochroite	-7.67	7.53	15.20	Mn(OH) ₂
Pyrolusite	-26.49	15.64	42.13	MnO ₂
Quartz	0.34	-3.71	-4.05	SiO ₂
Rhodochrosite	-0.04	-11.15	-11.11	MnCO ₃
Schwertmannite(1)	-47.12	-36.62	10.50	Fe ₈ O ₈ (OH) _{4.4} (SO ₄) _{1.8} ·8.4H ₂ O
Schwertmannite(2)	-42.40	-24.40	18.00	Fe ₈ O ₈ (OH) ₆ SO ₄
Sepiolite	-6.79	9.09	15.88	Mg ₂ Si ₃ O ₇ ·5OH·3H ₂ O
Sepiolite(d)	-9.57	9.09	18.66	Mg ₂ Si ₃ O ₇ ·5OH·3H ₂ O
Siderite	0.11	-10.75	-10.86	FeCO ₃
SiO ₂ (a)	-0.96	-3.71	-2.75	SiO ₂
Smithsonite	-2.68	-12.63	-9.95	ZnCO ₃
Sphalerite	4.42	-7.30	-11.71	ZnS
Strontianite	-1.17	-10.44	-9.27	SrCO ₃
Sulfur	-3.23	1.76	4.99	S
Talc	-6.44	15.50	21.93	Mg ₃ Si ₄ O ₁₀ (OH) ₂
Troilite	0.73	-5.42	-6.15	FeS
Willemite	-7.32	8.39	15.71	Zn ₂ SiO ₄
Witherite	-4.75	-13.32	-8.57	BaCO ₃
Zn(OH) ₂ (e)	-5.45	6.05	11.50	Zn(OH) ₂

End of simulation.

Reading input data for simulation 11.

SOLUTION 1 MP4 9-6-2007
temp 18.7
pH 6.48
pe 4
redox S(-2)/S(6)
units mg/kgw
density 1
Fe 3.8
S(6) 1870 as SO4
S(-2) 0.005
Cl 309
Br 1.4
Alkalinity 1400 as HCO3
Ba 0.012
Ca 596
Mg 135
Na 474
K 7.12
Mn 1.2
Si 9.74
Sr 6.69
Zn 0.1
water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. MP4 9-6-2007

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	2.294e-002	2.294e-002
Ba	8.737e-008	8.737e-008
Br	1.752e-005	1.752e-005
Ca	1.487e-002	1.487e-002
Cl	8.716e-003	8.716e-003
Fe	6.804e-005	6.804e-005
K	1.821e-004	1.821e-004
Mg	5.553e-003	5.553e-003
Mn	2.184e-005	2.184e-005
Na	2.062e-002	2.062e-002
S(-2)	1.559e-007	1.559e-007

S (6)	1.947e-002	1.947e-002
Si	1.621e-004	1.621e-004
Sr	7.635e-005	7.635e-005
Zn	1.530e-006	1.530e-006

-----Description of solution-----

pH	=	6.480
pe	=	4.000
Activity of water	=	0.998
Ionic strength	=	7.936e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	3.665e-002
Total CO2 (mol/kg)	=	3.665e-002
Temperature (deg C)	=	18.700
Electrical balance (eq)	=	-8.628e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	-8.18
Iterations	=	11
Total H	=	1.110360e+002
Total O	=	5.568095e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.3101	-0.1338

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.959e-007	3.311e-007	-6.402	-6.480	-0.078
OH-	2.361e-008	1.844e-008	-7.627	-7.734	-0.107
H2O	5.551e+001	9.983e-001	1.744	-0.001	0.000
Ba	8.737e-008				
BaSO4	4.386e-008	4.467e-008	-7.358	-7.350	0.008
Ba+2	4.069e-008	1.662e-008	-7.391	-7.779	-0.389
BaHCO3+	2.812e-009	2.240e-009	-8.551	-8.650	-0.099
BaCO3	1.572e-011	1.601e-011	-10.804	-10.796	0.008
BaOH+	2.132e-015	1.698e-015	-14.671	-14.770	-0.099
Br	1.752e-005				
Br-	1.752e-005	1.356e-005	-4.756	-4.868	-0.111
C(4)	3.665e-002				
HCO3-	2.132e-002	1.714e-002	-1.671	-1.766	-0.095
CO2	1.373e-002	1.398e-002	-1.862	-1.854	0.008
CaHCO3+	1.004e-003	8.068e-004	-2.998	-3.093	-0.095
MgHCO3+	3.804e-004	3.030e-004	-3.420	-3.519	-0.099
NaHCO3	1.508e-004	1.535e-004	-3.822	-3.814	0.008
FeHCO3+	2.727e-005	2.172e-005	-4.564	-4.663	-0.099
CaCO3	1.285e-005	1.309e-005	-4.891	-4.883	0.008
MnHCO3+	7.954e-006	6.336e-006	-5.099	-5.198	-0.099
SrHCO3+	5.614e-006	4.513e-006	-5.251	-5.346	-0.095
CO3-2	5.064e-006	2.115e-006	-5.295	-5.675	-0.379

		MgCO ₃	2.783e-006	2.835e-006	-5.555	-5.548	0.008
		MnCO ₃	6.842e-007	6.968e-007	-6.165	-6.157	0.008
		FeCO ₃	6.314e-007	6.430e-007	-6.200	-6.192	0.008
		ZnHCO ₃ +	5.964e-007	4.750e-007	-6.224	-6.323	-0.099
		NaCO ₃ -	5.693e-007	4.535e-007	-6.245	-6.343	-0.099
		ZnCO ₃	9.122e-008	9.290e-008	-7.040	-7.032	0.008
		SrCO ₃	2.351e-008	2.394e-008	-7.629	-7.621	0.008
		Zn (CO ₃) 2-2	1.044e-008	4.201e-009	-7.981	-8.377	-0.395
		Fe (CO ₃) (OH) -	9.468e-009	7.542e-009	-8.024	-8.123	-0.099
		Fe (CO ₃) 2-2	3.969e-009	1.598e-009	-8.401	-8.796	-0.395
		BaHCO ₃ +	2.812e-009	2.240e-009	-8.551	-8.650	-0.099
		BaCO ₃	1.572e-011	1.601e-011	-10.804	-10.796	0.008
Ca	1.487e-002						
		Ca+2	9.781e-003	4.118e-003	-2.010	-2.385	-0.376
		CaSO ₄	4.073e-003	4.148e-003	-2.390	-2.382	0.008
		CaHCO ₃ +	1.004e-003	8.068e-004	-2.998	-3.093	-0.095
		CaCO ₃	1.285e-005	1.309e-005	-4.891	-4.883	0.008
		CaHSO ₄ +	9.385e-009	7.475e-009	-8.028	-8.126	-0.099
		CaOH+	2.587e-009	2.061e-009	-8.587	-8.686	-0.099
Cl	8.716e-003						
		Cl-	8.715e-003	6.825e-003	-2.060	-2.166	-0.106
		FeCl+	1.499e-007	1.194e-007	-6.824	-6.923	-0.099
		MnCl+	1.448e-007	1.153e-007	-6.839	-6.938	-0.099
		ZnCl+	3.823e-009	3.045e-009	-8.418	-8.516	-0.099
		MnCl ₂	3.373e-010	3.436e-010	-9.472	-9.464	0.008
		ZnCl ₂	2.082e-011	2.121e-011	-10.681	-10.674	0.008
		MnCl ₃ -	8.108e-013	6.459e-013	-12.091	-12.190	-0.099
		ZnCl ₃ -	1.962e-013	1.562e-013	-12.707	-12.806	-0.099
		ZnCl ₄ -2	1.262e-015	5.079e-016	-14.899	-15.294	-0.395
		FeCl+2	1.739e-021	7.000e-022	-20.760	-21.155	-0.395
		FeCl ₂ +	3.286e-023	2.617e-023	-22.483	-22.582	-0.099
		FeCl ₃	1.754e-026	1.786e-026	-25.756	-25.748	0.008
Fe (2)	6.804e-005						
		Fe+2	2.941e-005	1.267e-005	-4.531	-4.897	-0.366
		FeHCO ₃ +	2.727e-005	2.172e-005	-4.564	-4.663	-0.099
		FeSO ₄	1.055e-005	1.074e-005	-4.977	-4.969	0.008
		FeCO ₃	6.314e-007	6.430e-007	-6.200	-6.192	0.008
		FeCl+	1.499e-007	1.194e-007	-6.824	-6.923	-0.099
		Fe (CO ₃) (OH) -	9.468e-009	7.542e-009	-8.024	-8.123	-0.099
		FeOH+	9.377e-009	7.470e-009	-8.028	-8.127	-0.099
		FeS	7.406e-009	7.543e-009	-8.130	-8.122	0.008
		Fe (CO ₃) 2-2	3.969e-009	1.598e-009	-8.401	-8.796	-0.395
		FeHSO ₄ +	2.888e-011	2.300e-011	-10.539	-10.638	-0.099
		Fe (HS) 2	1.082e-011	1.102e-011	-10.966	-10.958	0.008
		Fe (OH) 2	2.776e-013	2.828e-013	-12.557	-12.549	0.008
		Fe (HS) 3-	4.706e-017	3.748e-017	-16.327	-16.426	-0.099
Fe (3)	6.717e-014						
		Fe (OH) 2+	5.450e-014	4.341e-014	-13.264	-13.362	-0.099
		Fe (OH) 3	1.250e-014	1.274e-014	-13.903	-13.895	0.008
		FeOH+2	1.379e-016	5.550e-017	-15.861	-16.256	-0.395
		Fe (OH) 4-	3.394e-017	2.704e-017	-16.469	-16.568	-0.099
		FeSO ₄ +	2.666e-019	2.123e-019	-18.574	-18.673	-0.099
		Fe (SO ₄) 2-	3.049e-020	2.429e-020	-19.516	-19.615	-0.099
		Fe+3	2.080e-020	4.165e-021	-19.682	-20.380	-0.698

FeCl+2	1.739e-021	7.000e-022	-20.760	-21.155	-0.395
FeCl2+	3.286e-023	2.617e-023	-22.483	-22.582	-0.099
FeHSO4+2	4.717e-025	1.899e-025	-24.326	-24.721	-0.395
FeCl3	1.754e-026	1.786e-026	-25.756	-25.748	0.008
Fe2 (OH) 2+4	4.118e-030	1.082e-031	-29.385	-30.966	-1.581
Fe3 (OH) 4+5	5.240e-040	0.000e+000	-39.281	-41.750	-2.470
H (0)	6.779e-012				
H2	3.389e-012	3.452e-012	-11.470	-11.462	0.008
K	1.821e-004				
K+	1.763e-004	1.380e-004	-3.754	-3.860	-0.106
KSO4-	5.834e-006	4.647e-006	-5.234	-5.333	-0.099
KOH	1.417e-012	1.443e-012	-11.849	-11.841	0.008
Mg	5.553e-003				
Mg+2	3.552e-003	1.547e-003	-2.450	-2.810	-0.361
MgSO4	1.618e-003	1.647e-003	-2.791	-2.783	0.008
MgHCO3+	3.804e-004	3.030e-004	-3.420	-3.519	-0.099
MgCO3	2.783e-006	2.835e-006	-5.555	-5.548	0.008
MgOH+	5.131e-009	4.087e-009	-8.290	-8.389	-0.099
Mn (2)	2.184e-005				
Mn+2	9.626e-006	4.147e-006	-5.017	-5.382	-0.366
MnHCO3+	7.954e-006	6.336e-006	-5.099	-5.198	-0.099
MnSO4	3.434e-006	3.497e-006	-5.464	-5.456	0.008
MnCO3	6.842e-007	6.968e-007	-6.165	-6.157	0.008
MnCl+	1.448e-007	1.153e-007	-6.839	-6.938	-0.099
MnCl2	3.373e-010	3.436e-010	-9.472	-9.464	0.008
MnOH+	2.388e-010	1.902e-010	-9.622	-9.721	-0.099
MnCl3-	8.108e-013	6.459e-013	-12.091	-12.190	-0.099
Mn (3)	1.899e-033				
Mn+3	1.899e-033	2.451e-034	-32.722	-33.611	-0.889
Na	2.062e-002				
Na+	1.995e-002	1.593e-002	-1.700	-1.798	-0.098
NaSO4-	5.158e-004	4.109e-004	-3.287	-3.386	-0.099
NaHCO3	1.508e-004	1.535e-004	-3.822	-3.814	0.008
NaCO3-	5.693e-007	4.535e-007	-6.245	-6.343	-0.099
NaOH	3.115e-010	3.173e-010	-9.506	-9.499	0.008
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-71.543	-71.535	0.008
S (-2)	1.559e-007				
H2S	1.085e-007	1.105e-007	-6.965	-6.957	0.008
HS-	4.000e-008	3.124e-008	-7.398	-7.505	-0.107
FeS	7.406e-009	7.543e-009	-8.130	-8.122	0.008
Fe (HS) 2	1.082e-011	1.102e-011	-10.966	-10.958	0.008
S-2	1.795e-014	7.332e-015	-13.746	-14.135	-0.389
Fe (HS) 3-	4.706e-017	3.748e-017	-16.327	-16.426	-0.099
S (6)	1.947e-002				
SO4-2	1.322e-002	5.361e-003	-1.879	-2.271	-0.392
CaSO4	4.073e-003	4.148e-003	-2.390	-2.382	0.008
MgSO4	1.618e-003	1.647e-003	-2.791	-2.783	0.008
NaSO4-	5.158e-004	4.109e-004	-3.287	-3.386	-0.099
SrSO4	2.032e-005	2.070e-005	-4.692	-4.684	0.008
FeSO4	1.055e-005	1.074e-005	-4.977	-4.969	0.008
KSO4-	5.834e-006	4.647e-006	-5.234	-5.333	-0.099
MnSO4	3.434e-006	3.497e-006	-5.464	-5.456	0.008
ZnSO4	2.585e-007	2.633e-007	-6.587	-6.580	0.008

HSO4-	1.895e-007	1.510e-007	-6.722	-6.821	-0.099
BaSO4	4.386e-008	4.467e-008	-7.358	-7.350	0.008
Zn(SO4)2-2	2.995e-008	1.206e-008	-7.524	-7.919	-0.395
CaHSO4+	9.385e-009	7.475e-009	-8.028	-8.126	-0.099
FeHSO4+	2.888e-011	2.300e-011	-10.539	-10.638	-0.099
FeSO4+	2.666e-019	2.123e-019	-18.574	-18.673	-0.099
Fe(SO4)2-	3.049e-020	2.429e-020	-19.516	-19.615	-0.099
FeHSO4+2	4.717e-025	1.899e-025	-24.326	-24.721	-0.395
Si	1.621e-004				
H4SiO4	1.620e-004	1.650e-004	-3.790	-3.782	0.008
H3SiO4-	7.342e-008	5.848e-008	-7.134	-7.233	-0.099
H2SiO4-2	1.949e-014	7.846e-015	-13.710	-14.105	-0.395
Sr	7.635e-005				
Sr+2	5.039e-005	2.136e-005	-4.298	-4.670	-0.373
SrSO4	2.032e-005	2.070e-005	-4.692	-4.684	0.008
SrHCO3+	5.614e-006	4.513e-006	-5.251	-5.346	-0.095
SrCO3	2.351e-008	2.394e-008	-7.629	-7.621	0.008
SrOH+	4.130e-012	3.302e-012	-11.384	-11.481	-0.097
Zn	1.530e-006				
ZnHCO3+	5.964e-007	4.750e-007	-6.224	-6.323	-0.099
Zn+2	5.388e-007	2.201e-007	-6.269	-6.657	-0.389
ZnSO4	2.585e-007	2.633e-007	-6.587	-6.580	0.008
ZnCO3	9.122e-008	9.290e-008	-7.040	-7.032	0.008
Zn(SO4)2-2	2.995e-008	1.206e-008	-7.524	-7.919	-0.395
Zn(CO3)2-2	1.044e-008	4.201e-009	-7.981	-8.377	-0.395
ZnCl+	3.823e-009	3.045e-009	-8.418	-8.516	-0.099
ZnOH+	5.607e-010	4.466e-010	-9.251	-9.350	-0.099
Zn(OH)2	2.473e-011	2.519e-011	-10.607	-10.599	0.008
ZnCl2	2.082e-011	2.121e-011	-10.681	-10.674	0.008
ZnCl3-	1.962e-013	1.562e-013	-12.707	-12.806	-0.099
ZnCl4-2	1.262e-015	5.079e-016	-14.899	-15.294	-0.395
Zn(OH)3-	3.015e-016	2.402e-016	-15.521	-15.619	-0.099
Zn(OH)4-2	2.851e-022	1.148e-022	-21.545	-21.940	-0.395

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH)5]	-2.80	20.29	23.09	Fe2(OH)5
[Fe3(OH)7]	3.36	28.35	24.99	Fe3(OH)7
[Fe3(OH)8]	-9.60	32.52	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-20.28	38.07	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-18.90	41.48	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-15.79	27.77	43.56	Fe4(OH)8(Cl)1
Anhydrite	-0.32	-4.66	-4.34	CaSO4
Aragonite	0.24	-8.06	-8.30	CaCO3
Barite	0.03	-10.05	-10.08	BaSO4
Brucite	-6.64	10.15	16.79	Mg(OH)2
Calcite	0.39	-8.06	-8.45	CaCO3
Celestite	-0.32	-6.94	-6.62	SrSO4
Chalcedony	-0.15	-3.78	-3.63	SiO2
Chrysotile	-10.12	22.88	33.00	Mg3Si2O5(OH)4
CO2(g)	-0.46	-1.85	-1.39	CO2
Dolomite	0.40	-16.55	-16.94	CaMg(CO3)2

Epsomite	-2.90	-5.09	-2.18	MgSO4:7H2O
Fe (OH) 2 (1)	-4.88	8.06	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-5.83	8.06	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-5.83	-0.94	4.89	Fe (OH) 3
FeO	-5.53	8.06	13.59	FeO
FeS (am)	-2.08	-5.92	-3.84	FeS
FeS (ppt)	-2.01	-5.92	-3.92	FeS
Goethite	-0.17	-0.94	-0.77	FeOOH
Greigite	-11.13	-49.76	-38.63	Fe3S4
Gypsum	-0.08	-4.66	-4.58	CaSO4:2H2O
H2 (g)	-8.34	-11.46	-3.12	H2
H2O (g)	-1.68	-0.00	1.68	H2O
H2S (g)	-6.03	-6.96	-0.92	H2S
Halite	-5.53	-3.96	1.57	NaCl
Hausmannite	-31.55	31.07	62.62	Mn3O4
Hematite	1.64	-1.88	-3.52	Fe2O3
Jarosite-H3O	-22.05	-33.29	-11.24	H3OFe3 (SO4) 2 (OH) 6
Jarosite-K	-19.84	-30.67	-10.83	KFe3 (SO4) 2 (OH) 6
Lepidocrocite	-4.47	12.23	16.70	FeOOH
Lime	-12.24	10.57	22.81	Ca (OH) 2
Mackinawite	-1.34	-5.92	-4.58	FeS
Mackinawite (2)	-2.39	1.11	3.50	FeS
Magnetite	-13.27	32.53	45.80	Fe3O4
Manganite	-13.59	11.75	25.34	MnOOH
Marcasite	6.36	-11.57	-17.93	FeS2
Melanterite	-4.88	-7.17	-2.29	FeSO4:7H2O
Nesquehonite	-2.96	-8.49	-5.53	MgCO3:3H2O
O2 (g)	-68.60	-71.53	-2.93	O2
Pyrite	7.09	-11.57	-18.66	FeS2
Pyrochroite	-7.62	7.58	15.20	Mn (OH) 2
Pyrolusite	-26.49	15.92	42.41	MnO2
Quartz	0.29	-3.78	-4.08	SiO2
Rhodochrosite	0.05	-11.06	-11.11	MnCO3
Schwertmannite (1)	-45.45	-34.95	10.50	Fe8O8 (OH) 4.4 (SO4) 1.8:8.4H2O
Schwertmannite (2)	-40.76	-22.76	18.00	Fe8O8 (OH) 6SO4
Sepiolite	-6.98	8.95	15.93	Mg2Si3O7.5OH:3H2O
Sepiolite (d)	-9.71	8.95	18.66	Mg2Si3O7.5OH:3H2O
Siderite	0.28	-10.57	-10.85	FeCO3
SiO2 (a)	-1.02	-3.78	-2.76	SiO2
Smithsonite	-2.40	-12.33	-9.93	ZnCO3
Sphalerite	4.07	-7.68	-11.75	ZnS
Strontianite	-1.08	-10.35	-9.27	SrCO3
Sulfur	-3.65	1.38	5.03	S
Talc	-6.81	15.32	22.13	Mg3Si4O10 (OH) 2
Troilite	0.22	-5.92	-6.14	FeS
Willemite	-7.04	8.82	15.86	Zn2SiO4
Witherite	-4.87	-13.45	-8.58	BaCO3
Zn (OH) 2 (e)	-5.20	6.30	11.50	Zn (OH) 2

End of simulation.

Reading input data for simulation 12.

End of run.

EPA Column Study (Altus SS-17)

Input file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\EPA_Column.pqi
Output file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\EPA_Column.pqi
Database file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\phreeqc8.dat

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\phreeqc8.dat

SOLUTION 1 EPA Column B3E 5/15/07

temp	22.3
pH	7.35
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
S(-2)	7.79
S(6)	1670 as SO4
Ba	0.161
Ca	436
K	9.31
Mg	183
B	5.26
Al	0.154
Na	790
Sr	7.71
Zn	0.05
Alkalinity	689 as CaCO3
Fe	0.04
Cl	812
water	1 # kg

Beginning of initial solution calculations.

Initial solution 1. EPA Column B3E 5/15/07

WARNING: Equivalent wt for alkalinity should be $\text{Ca} \cdot 5(\text{CO}_3) \cdot 5$. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Al	5.708e-006	5.708e-006
Alkalinity	1.377e-002	1.377e-002
B	4.866e-004	4.866e-004
Ba	1.172e-006	1.172e-006
Ca	1.088e-002	1.088e-002
Cl	2.290e-002	2.290e-002
Fe	7.162e-007	7.162e-007
K	2.381e-004	2.381e-004
Mg	7.527e-003	7.527e-003
Na	3.436e-002	3.436e-002
S(-2)	2.430e-004	2.430e-004
S(6)	1.738e-002	1.738e-002
Sr	8.799e-005	8.799e-005
Zn	7.649e-007	7.649e-007

-----Description of solution-----

pH	=	7.350
pe	=	4.000
Activity of water	=	0.998
Ionic strength	=	8.422e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	1.447e-002
Total CO2 (mol/kg)	=	1.447e-002
Temperature (deg C)	=	22.300
Electrical balance (eq)	=	1.709e-004
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	0.14
Iterations	=	9
Total H	=	1.110276e+002
Total O	=	5.561963e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-3.8226	-0.2241

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	2.345e-007	1.819e-007	-6.630	-6.740	-0.110
H+	5.361e-008	4.467e-008	-7.271	-7.350	-0.079
H2O	5.551e+001	9.983e-001	1.744	-0.001	0.000
Al	5.708e-006				
Al(OH)4-	5.550e-006	4.396e-006	-5.256	-5.357	-0.101
Al(OH)3	1.060e-007	1.081e-007	-6.975	-6.966	0.008

	Al (OH) 2+	5.071e-008	4.017e-008	-7.295	-7.396	-0.101
	AlOH+2	7.402e-010	2.914e-010	-9.131	-9.536	-0.405
	AlSO4+	2.794e-011	2.213e-011	-10.554	-10.655	-0.101
	Al+3	8.094e-012	1.566e-012	-11.092	-11.805	-0.713
	Al (SO4) 2-	4.038e-012	3.199e-012	-11.394	-11.495	-0.101
	AlHSO4+2	2.176e-019	8.566e-020	-18.662	-19.067	-0.405
B		4.866e-004				
	H3BO3	4.790e-004	4.884e-004	-3.320	-3.311	0.008
	H2BO3-	7.558e-006	5.987e-006	-5.122	-5.223	-0.101
Ba		1.172e-006				
	Ba+2	5.998e-007	2.395e-007	-6.222	-6.621	-0.399
	BaSO4	5.449e-007	5.555e-007	-6.264	-6.255	0.008
	BaHCO3+	2.643e-008	2.094e-008	-7.578	-7.679	-0.101
	BaCO3	1.132e-009	1.155e-009	-8.946	-8.938	0.008
	BaOH+	2.289e-013	1.813e-013	-12.640	-12.742	-0.101
C (4)		1.447e-002				
	HCO3-	1.242e-002	9.930e-003	-1.906	-2.003	-0.097
	CO2	1.015e-003	1.035e-003	-2.993	-2.985	0.008
	CaHCO3+	4.747e-004	3.795e-004	-3.324	-3.421	-0.097
	MgHCO3+	3.130e-004	2.480e-004	-3.504	-3.606	-0.101
	NaHCO3	1.454e-004	1.483e-004	-3.837	-3.829	0.008
	CaCO3	4.825e-005	4.920e-005	-4.316	-4.308	0.008
	CO3-2	2.412e-005	9.854e-006	-4.618	-5.006	-0.389
	MgCO3	1.910e-005	1.947e-005	-4.719	-4.711	0.008
	NaCO3-	5.361e-006	4.246e-006	-5.271	-5.372	-0.101
	SrHCO3+	4.423e-006	3.536e-006	-5.354	-5.452	-0.097
	ZnCO3	1.778e-007	1.813e-007	-6.750	-6.742	0.008
	ZnHCO3+	1.455e-007	1.153e-007	-6.837	-6.938	-0.101
	SrCO3	1.455e-007	1.483e-007	-6.837	-6.829	0.008
	Zn (CO3) 2-2	9.702e-008	3.819e-008	-7.013	-7.418	-0.405
	BaHCO3+	2.643e-008	2.094e-008	-7.578	-7.679	-0.101
	FeHCO3+	2.123e-008	1.681e-008	-7.673	-7.774	-0.101
	FeCO3	3.926e-009	4.002e-009	-8.406	-8.398	0.008
	BaCO3	1.132e-009	1.155e-009	-8.946	-8.938	0.008
	Fe (CO3) (OH) -	4.393e-010	3.480e-010	-9.357	-9.458	-0.101
	Fe (CO3) 2-2	1.177e-010	4.634e-011	-9.929	-10.334	-0.405
Ca		1.088e-002				
	Ca+2	7.592e-003	3.129e-003	-2.120	-2.505	-0.385
	CaSO4	2.763e-003	2.818e-003	-2.559	-2.550	0.008
	CaHCO3+	4.747e-004	3.795e-004	-3.324	-3.421	-0.097
	CaCO3	4.825e-005	4.920e-005	-4.316	-4.308	0.008
	CaOH+	1.465e-008	1.161e-008	-7.834	-7.935	-0.101
	CaHSO4+	9.008e-010	7.135e-010	-9.045	-9.147	-0.101
Cl		2.290e-002				
	Cl-	2.290e-002	1.782e-002	-1.640	-1.749	-0.109
	ZnCl+	4.950e-009	3.921e-009	-8.305	-8.407	-0.101
	FeCl+	5.257e-010	4.164e-010	-9.279	-9.380	-0.101
	ZnCl2	7.095e-011	7.234e-011	-10.149	-10.141	0.008
	ZnCl3-	1.796e-012	1.423e-012	-11.746	-11.847	-0.101
	ZnCl4-2	3.158e-014	1.243e-014	-13.501	-13.906	-0.405
	FeCl+2	2.627e-025	1.034e-025	-24.580	-24.985	-0.405
	FeCl2+	1.133e-026	8.972e-027	-25.946	-26.047	-0.101
	FeCl3	1.568e-029	1.598e-029	-28.805	-28.796	0.008
Fe (2)		7.162e-007				

FeS	3.328e-007	3.394e-007	-6.478	-6.469	0.008
Fe (HS) 2	2.980e-007	3.038e-007	-6.526	-6.517	0.008
Fe+2	4.012e-008	1.693e-008	-7.397	-7.771	-0.375
FeHCO3+	2.123e-008	1.681e-008	-7.673	-7.774	-0.101
FeSO4	1.301e-008	1.326e-008	-7.886	-7.877	0.008
Fe (HS) 3-	5.926e-009	4.694e-009	-8.227	-8.328	-0.101
FeCO3	3.926e-009	4.002e-009	-8.406	-8.398	0.008
FeCl+	5.257e-010	4.164e-010	-9.279	-9.380	-0.101
Fe (CO3) (OH) -	4.393e-010	3.480e-010	-9.357	-9.458	-0.101
FeOH+	1.232e-010	9.762e-011	-9.909	-10.010	-0.101
Fe (CO3) 2-2	1.177e-010	4.634e-011	-9.929	-10.334	-0.405
Fe (OH) 2	2.036e-014	2.076e-014	-13.691	-13.683	0.008
FeHSO4+	4.874e-015	3.861e-015	-14.312	-14.413	-0.101
Fe (3)	6.582e-016				
Fe (OH) 3	4.310e-016	4.395e-016	-15.365	-15.357	0.008
Fe (OH) 2+	2.170e-016	1.719e-016	-15.664	-15.765	-0.101
Fe (OH) 4-	1.014e-017	8.028e-018	-16.994	-17.095	-0.101
FeOH+2	6.543e-020	2.576e-020	-19.184	-19.589	-0.405
FeSO4+	1.264e-023	1.001e-023	-22.898	-22.999	-0.101
Fe (SO4) 2-	1.267e-024	1.003e-024	-23.897	-23.999	-0.101
Fe+3	1.083e-024	2.096e-025	-23.965	-24.679	-0.713
FeCl+2	2.627e-025	1.034e-025	-24.580	-24.985	-0.405
FeCl2+	1.133e-026	8.972e-027	-25.946	-26.047	-0.101
FeCl3	1.568e-029	1.598e-029	-28.805	-28.796	0.008
FeHSO4+2	3.049e-030	1.200e-030	-29.516	-29.921	-0.405
Fe2 (OH) 2+4	8.324e-037	1.998e-038	-36.080	-37.699	-1.620
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-48.504	-51.035	-2.531
H (0)	1.258e-010				
H2	6.288e-011	6.411e-011	-10.201	-10.193	0.008
K	2.381e-004				
K+	2.311e-004	1.797e-004	-3.636	-3.745	-0.109
KSO4-	7.037e-006	5.574e-006	-5.153	-5.254	-0.101
KOH	1.366e-011	1.393e-011	-10.865	-10.856	0.008
Mg	7.527e-003				
Mg+2	5.054e-003	2.158e-003	-2.296	-2.666	-0.370
MgSO4	2.141e-003	2.183e-003	-2.669	-2.661	0.008
MgHCO3+	3.130e-004	2.480e-004	-3.504	-3.606	-0.101
MgCO3	1.910e-005	1.947e-005	-4.719	-4.711	0.008
MgOH+	7.460e-008	5.909e-008	-7.127	-7.229	-0.101
Na	3.436e-002				
Na+	3.345e-002	2.655e-002	-1.476	-1.576	-0.100
NaSO4-	7.644e-004	6.055e-004	-3.117	-3.218	-0.101
NaHCO3	1.454e-004	1.483e-004	-3.837	-3.829	0.008
NaCO3-	5.361e-006	4.246e-006	-5.271	-5.372	-0.101
NaOH	3.845e-009	3.921e-009	-8.415	-8.407	0.008
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-72.883	-72.875	0.008
S (-2)	2.430e-004				
HS-	1.829e-004	1.419e-004	-3.738	-3.848	-0.110
H2S	5.906e-005	6.022e-005	-4.229	-4.220	0.008
FeS	3.328e-007	3.394e-007	-6.478	-6.469	0.008
Fe (HS) 2	2.980e-007	3.038e-007	-6.526	-6.517	0.008
Fe (HS) 3-	5.926e-009	4.694e-009	-8.227	-8.328	-0.101
S-2	7.974e-010	3.183e-010	-9.098	-9.497	-0.399

S (6)	1.738e-002					
SO4-2	1.169e-002	4.629e-003	-1.932	-2.335	-0.402	
CaSO4	2.763e-003	2.818e-003	-2.559	-2.550	0.008	
MgSO4	2.141e-003	2.183e-003	-2.669	-2.661	0.008	
NaSO4-	7.644e-004	6.055e-004	-3.117	-3.218	-0.101	
SrSO4	2.189e-005	2.232e-005	-4.660	-4.651	0.008	
KSO4-	7.037e-006	5.574e-006	-5.153	-5.254	-0.101	
BaSO4	5.449e-007	5.555e-007	-6.264	-6.255	0.008	
ZnSO4	9.609e-008	9.798e-008	-7.017	-7.009	0.008	
HSO4-	2.394e-008	1.896e-008	-7.621	-7.722	-0.101	
FeSO4	1.301e-008	1.326e-008	-7.886	-7.877	0.008	
Zn (SO4) 2-2	9.564e-009	3.764e-009	-8.019	-8.424	-0.405	
CaHSO4+	9.008e-010	7.135e-010	-9.045	-9.147	-0.101	
AlSO4+	2.794e-011	2.213e-011	-10.554	-10.655	-0.101	
Al (SO4) 2-	4.038e-012	3.199e-012	-11.394	-11.495	-0.101	
FeHSO4+	4.874e-015	3.861e-015	-14.312	-14.413	-0.101	
AlHSO4+2	2.176e-019	8.566e-020	-18.662	-19.067	-0.405	
FeSO4+	1.264e-023	1.001e-023	-22.898	-22.999	-0.101	
Fe (SO4) 2-	1.267e-024	1.003e-024	-23.897	-23.999	-0.101	
FeHSO4+2	3.049e-030	1.200e-030	-29.516	-29.921	-0.405	
Sr	8.799e-005					
Sr+2	6.154e-005	2.553e-005	-4.211	-4.593	-0.382	
SrSO4	2.189e-005	2.232e-005	-4.660	-4.651	0.008	
SrHCO3+	4.423e-006	3.536e-006	-5.354	-5.452	-0.097	
SrCO3	1.455e-007	1.483e-007	-6.837	-6.829	0.008	
SrOH+	3.682e-011	2.926e-011	-10.434	-10.534	-0.100	
Zn	7.649e-007					
Zn+2	2.310e-007	9.220e-008	-6.636	-7.035	-0.399	
ZnCO3	1.778e-007	1.813e-007	-6.750	-6.742	0.008	
ZnHCO3+	1.455e-007	1.153e-007	-6.837	-6.938	-0.101	
Zn (CO3) 2-2	9.702e-008	3.819e-008	-7.013	-7.418	-0.405	
ZnSO4	9.609e-008	9.798e-008	-7.017	-7.009	0.008	
Zn (SO4) 2-2	9.564e-009	3.764e-009	-8.019	-8.424	-0.405	
ZnCl+	4.950e-009	3.921e-009	-8.305	-8.407	-0.101	
ZnOH+	2.320e-009	1.838e-009	-8.635	-8.736	-0.101	
Zn (OH) 2	5.686e-010	5.798e-010	-9.245	-9.237	0.008	
ZnCl2	7.095e-011	7.234e-011	-10.149	-10.141	0.008	
ZnCl3-	1.796e-012	1.423e-012	-11.746	-11.847	-0.101	
Zn (OH) 3-	5.173e-014	4.097e-014	-13.286	-13.388	-0.101	
ZnCl4-2	3.158e-014	1.243e-014	-13.501	-13.906	-0.405	
Zn (OH) 4-2	3.687e-019	1.451e-019	-18.433	-18.838	-0.405	

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-5.71	17.38	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	-0.68	24.31	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-14.29	27.83	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-29.44	28.91	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-28.80	31.58	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-21.42	22.14	43.56	Fe4 (OH) 8 (Cl) 1
Al (OH) 3 (a)	-0.73	10.24	10.98	Al (OH) 3
Alunite	1.33	0.27	-1.06	KAl3 (SO4) 2 (OH) 6

Anhydrite	-0.49	-4.84	-4.35	CaSO4
Aragonite	0.81	-7.51	-8.32	CaCO3
Barite	1.06	-8.96	-10.01	BaSO4
Basaluminite	1.24	23.94	22.70	Al4(OH)10SO4
Brucite	-4.76	12.03	16.79	Mg(OH)2
Calcite	0.95	-7.51	-8.47	CaCO3
Celestite	-0.30	-6.93	-6.63	SrSO4
CO2(g)	-1.55	-2.99	-1.44	CO2
Dolomite	1.84	-15.18	-17.03	CaMg(CO3)2
Epsomite	-2.85	-5.01	-2.16	MgSO4·7H2O
Fe(OH)2(1)	-6.01	6.93	12.94	Fe(OH)2
Fe(OH)2(2)	-6.96	6.93	13.89	Fe(OH)2
Fe(OH)3(a)	-7.52	-2.63	4.89	Fe(OH)3
FeO	-6.66	6.93	13.59	FeO
FeS(am)	-0.39	-4.27	-3.88	FeS
FeS(ppt)	-0.35	-4.27	-3.92	FeS
Gibbsite	1.98	10.24	8.26	Al(OH)3
Goethite	-1.73	-2.63	-0.90	FeOOH
Greigite	-4.41	-43.12	-38.71	Fe3S4
Gypsum	-0.26	-4.84	-4.58	CaSO4·2H2O
H2(g)	-7.05	-10.19	-3.14	H2
H2O(g)	-1.58	-0.00	1.58	H2O
H2S(g)	-3.25	-4.22	-0.97	H2S
Halite	-4.90	-3.33	1.58	NaCl
Hematite	-1.46	-5.26	-3.80	Fe2O3
Jarosite-H3O	-30.22	-41.96	-11.74	H3OFe3(SO4)2(OH)6
Jarosite-K	-27.43	-38.36	-10.93	KFe3(SO4)2(OH)6
Jurbanite	-3.56	-6.79	-3.23	AlOHSO4
Lepidocrocite	-6.25	10.45	16.70	FeOOH
Lime	-10.62	12.19	22.81	Ca(OH)2
Mackinawite	0.35	-4.27	-4.62	FeS
Mackinawite(2)	-0.79	2.71	3.50	FeS
Magnetite	-17.96	27.84	45.80	Fe3O4
Marcasite	9.42	-8.41	-17.83	FeS2
Melanterite	-7.87	-10.11	-2.24	FeSO4·7H2O
Nesquehonite	-2.09	-7.67	-5.58	MgCO3·3H2O
O2(g)	-69.93	-72.87	-2.95	O2
Pyrite	10.14	-8.41	-18.55	FeS2
Schwertmannite(1)	-62.21	-51.71	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-56.07	-38.07	18.00	Fe8O8(OH)6SO4
Siderite	-1.90	-12.78	-10.87	FeCO3
Smithsonite	-2.07	-12.04	-9.97	ZnCO3
Sphalerite	8.14	-3.53	-11.67	ZnS
Strontianite	-0.33	-9.60	-9.27	SrCO3
Sulfur	-2.11	2.83	4.95	S
Troilite	1.88	-4.27	-6.15	FeS
Witherite	-3.06	-11.63	-8.57	BaCO3
Zn(OH)2(e)	-3.84	7.66	11.50	Zn(OH)2

End of simulation.

Reading input data for simulation 2.

End of run.

Dover AFB

Input file: C:\Documents and Settings\whitingks\My Documents\Program Files\USGS\Phreeqc Interactive 2.6\Dover.pqi

Output file: C:\Documents and Settings\whitingks\My Documents\Program Files\USGS\Phreeqc Interactive 2.6\Dover.pgo

Database file: C:\Documents and Settings\whitingks\My Documents\Program Files\USGS\Phreeqc Interactive 2.6\phreeqc8.dat

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Documents and Settings\whitingks\My Documents\Program Files\USGS\Phreeqc Interactive 2.6\phreeqc8.dat

SOLUTION 1 TS-MW11 3-18-2008 (Upgradient)

temp	12.5
pH	5.27
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	9.4
F	0.48
S(6)	6.4 as SO4
S(-2)	0.5
Ca	3.4
Fe(2)	1.1
Mg	2.1
Mn	0.031
K	0.78
Na	11
Alkalinity	18.7 as CaCO3
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. TS-MW11 3-18-2008 (Upgradient)

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	3.737e-004	3.737e-004
Ca	8.483e-005	8.483e-005
Cl	2.651e-004	2.651e-004
F	2.527e-005	2.527e-005
Fe (2)	1.970e-005	1.970e-005
K	1.995e-005	1.995e-005
Mg	8.638e-005	8.638e-005
Mn	5.643e-007	5.643e-007
Na	4.785e-004	4.785e-004
S (-2)	1.559e-005	1.559e-005
S (6)	6.662e-005	6.662e-005

-----Description of solution-----

pH	=	5.270
pe	=	4.000
Activity of water	=	1.000
Ionic strength	=	1.094e-003
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	5.771e-003
Total CO2 (mol/kg)	=	5.771e-003
Temperature (deg C)	=	12.500
Electrical balance (eq)	=	8.405e-005
Percent error, 100*(Cat- An)/(Cat+ An)	=	5.00
Iterations	=	8
Total H	=	1.110128e+002
Total O	=	5.551840e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2)/S (6)	-1.1792	-0.0668

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.560e-006	5.370e-006	-5.255	-5.270	-0.015
OH-	7.034e-010	6.781e-010	-9.153	-9.169	-0.016
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
C (4)	5.771e-003				
CO2	5.392e-003	5.393e-003	-2.268	-2.268	0.000
HCO3-	3.778e-004	3.645e-004	-3.423	-3.438	-0.016
FeHCO3+	6.205e-007	5.983e-007	-6.207	-6.223	-0.016
MgHCO3+	3.145e-007	3.033e-007	-6.502	-6.518	-0.016
CaHCO3+	2.725e-007	2.629e-007	-6.565	-6.580	-0.016
NaHCO3	9.452e-008	9.454e-008	-7.024	-7.024	0.000
MnHCO3+	1.589e-008	1.532e-008	-7.799	-7.815	-0.016

	CO3-2	2.734e-009	2.368e-009	-8.563	-8.626	-0.062
	FeCO3	9.322e-010	9.325e-010	-9.030	-9.030	0.000
	CaCO3	2.395e-010	2.395e-010	-9.621	-9.621	0.000
	MgCO3	1.378e-010	1.378e-010	-9.861	-9.861	0.000
	MnCO3	8.869e-011	8.872e-011	-10.052	-10.052	0.000
	NaCO3-	1.092e-011	1.053e-011	-10.962	-10.977	-0.016
	Fe (CO3) (OH) -	7.005e-013	6.754e-013	-12.155	-12.170	-0.016
	Fe (CO3) 2-2	3.001e-015	2.595e-015	-14.523	-14.586	-0.063
Ca	8.483e-005					
	Ca+2	8.383e-005	7.259e-005	-4.077	-4.139	-0.062
	CaSO4	7.203e-007	7.205e-007	-6.142	-6.142	0.000
	CaHCO3+	2.725e-007	2.629e-007	-6.565	-6.580	-0.016
	CaF+	1.165e-008	1.124e-008	-7.934	-7.949	-0.016
	CaCO3	2.395e-010	2.395e-010	-9.621	-9.621	0.000
	CaHSO4+	2.052e-011	1.978e-011	-10.688	-10.704	-0.016
	CaOH+	2.326e-012	2.243e-012	-11.633	-11.649	-0.016
Cl	2.651e-004					
	Cl-	2.651e-004	2.556e-004	-3.577	-3.592	-0.016
	FeCl+	6.006e-009	5.792e-009	-8.221	-8.237	-0.016
	MnCl+	5.093e-010	4.911e-010	-9.293	-9.309	-0.016
	MnCl2	5.478e-014	5.479e-014	-13.261	-13.261	0.000
	MnCl3-	4.000e-018	3.857e-018	-17.398	-17.414	-0.016
F	2.527e-005					
	F-	2.499e-005	2.409e-005	-4.602	-4.618	-0.016
	HF	1.558e-007	1.559e-007	-6.807	-6.807	0.000
	MgF+	9.632e-008	9.287e-008	-7.016	-7.032	-0.016
	CaF+	1.165e-008	1.124e-008	-7.934	-7.949	-0.016
	NaF	6.392e-009	6.394e-009	-8.194	-8.194	0.000
	FeF+	4.101e-009	3.955e-009	-8.387	-8.403	-0.016
	MnF+	8.152e-011	7.861e-011	-10.089	-10.105	-0.016
	HF2-	1.329e-011	1.282e-011	-10.876	-10.892	-0.016
Fe (2)	1.970e-005					
	Fe+2	1.893e-005	1.641e-005	-4.723	-4.785	-0.062
	FeHCO3+	6.205e-007	5.983e-007	-6.207	-6.223	-0.016
	FeSO4	1.292e-007	1.292e-007	-6.889	-6.889	0.000
	FeCl+	6.006e-009	5.792e-009	-8.221	-8.237	-0.016
	FeF+	4.101e-009	3.955e-009	-8.387	-8.403	-0.016
	FeCO3	9.322e-010	9.325e-010	-9.030	-9.030	0.000
	Fe (HS) 2	6.750e-010	6.751e-010	-9.171	-9.171	0.000
	FeOH+	3.781e-010	3.646e-010	-9.422	-9.438	-0.016
	FeHSO4+	4.639e-012	4.473e-012	-11.334	-11.349	-0.016
	Fe (CO3) (OH) -	7.005e-013	6.754e-013	-12.155	-12.170	-0.016
	Fe (HS) 3-	1.638e-014	1.579e-014	-13.786	-13.802	-0.016
	Fe (CO3) 2-2	3.001e-015	2.595e-015	-14.523	-14.586	-0.063
	Fe (OH) 2	1.396e-015	1.397e-015	-14.855	-14.855	0.000
H (0)	1.061e-011					
	H2	5.304e-012	5.305e-012	-11.275	-11.275	0.000
K	1.995e-005					
	K+	1.994e-005	1.922e-005	-4.700	-4.716	-0.016
	KSO4-	6.269e-009	6.045e-009	-8.203	-8.219	-0.016
	KOH	1.241e-014	1.241e-014	-13.906	-13.906	0.000
Mg	8.638e-005					
	Mg+2	8.527e-005	7.390e-005	-4.069	-4.131	-0.062
	MgSO4	6.955e-007	6.956e-007	-6.158	-6.158	0.000

MgHCO3+	3.145e-007	3.033e-007	-6.502	-6.518	-0.016
MgF+	9.632e-008	9.287e-008	-7.016	-7.032	-0.016
MgCO3	1.378e-010	1.378e-010	-9.861	-9.861	0.000
MgOH+	6.883e-012	6.637e-012	-11.162	-11.178	-0.016
Mn (2)	5.643e-007				
Mn+2	5.440e-007	4.716e-007	-6.264	-6.326	-0.062
MnHCO3+	1.589e-008	1.532e-008	-7.799	-7.815	-0.016
MnSO4	3.673e-009	3.674e-009	-8.435	-8.435	0.000
MnCl+	5.093e-010	4.911e-010	-9.293	-9.309	-0.016
MnCO3	8.869e-011	8.872e-011	-10.052	-10.052	0.000
MnF+	8.152e-011	7.861e-011	-10.089	-10.105	-0.016
MnOH+	8.081e-013	7.792e-013	-12.093	-12.108	-0.016
MnCl2	5.478e-014	5.479e-014	-13.261	-13.261	0.000
MnCl3-	4.000e-018	3.857e-018	-17.398	-17.414	-0.016
Mn (3)	1.992e-034				
Mn+3	1.992e-034	1.435e-034	-33.701	-33.843	-0.142
Na	4.785e-004				
Na+	4.782e-004	4.612e-004	-3.320	-3.336	-0.016
NaSO4-	1.240e-007	1.196e-007	-6.907	-6.922	-0.016
NaHCO3	9.452e-008	9.454e-008	-7.024	-7.024	0.000
NaF	6.392e-009	6.394e-009	-8.194	-8.194	0.000
NaCO3-	1.092e-011	1.053e-011	-10.962	-10.977	-0.016
NaOH	5.672e-013	5.674e-013	-12.246	-12.246	0.000
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-74.040	-74.040	0.000
S (-2)	1.559e-005				
H2S	1.537e-005	1.537e-005	-4.813	-4.813	0.000
HS-	2.228e-007	2.148e-007	-6.652	-6.668	-0.016
Fe (HS) 2	6.750e-010	6.751e-010	-9.171	-9.171	0.000
Fe (HS) 3-	1.638e-014	1.579e-014	-13.786	-13.802	-0.016
S-2	2.284e-015	1.977e-015	-14.641	-14.704	-0.063
S (6)	6.662e-005				
SO4-2	6.492e-005	5.619e-005	-4.188	-4.250	-0.063
CaSO4	7.203e-007	7.205e-007	-6.142	-6.142	0.000
MgSO4	6.955e-007	6.956e-007	-6.158	-6.158	0.000
FeSO4	1.292e-007	1.292e-007	-6.889	-6.889	0.000
NaSO4-	1.240e-007	1.196e-007	-6.907	-6.922	-0.016
HSO4-	2.351e-008	2.267e-008	-7.629	-7.645	-0.016
KSO4-	6.269e-009	6.045e-009	-8.203	-8.219	-0.016
MnSO4	3.673e-009	3.674e-009	-8.435	-8.435	0.000
CaHSO4+	2.052e-011	1.978e-011	-10.688	-10.704	-0.016
FeHSO4+	4.639e-012	4.473e-012	-11.334	-11.349	-0.016

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-7.49	15.60	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	-3.63	21.36	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-16.67	25.45	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-34.80	23.55	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-32.46	27.92	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-25.31	18.25	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-4.06	-8.39	-4.33	CaSO4

Aragonite	-4.50	-12.76	-8.27	CaCO3
Brucite	-10.38	6.41	16.79	Mg (OH) 2
Calcite	-4.34	-12.76	-8.42	CaCO3
CO2 (g)	-0.96	-2.27	-1.31	CO2
Dolomite	-8.73	-25.52	-16.79	CaMg (CO3) 2
Epsomite	-6.15	-8.38	-2.23	MgSO4:7H2O
Fe (OH) 2 (1)	-7.18	5.76	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-8.13	5.76	13.89	Fe (OH) 2
FeO	-7.83	5.76	13.59	FeO
FeS (am)	-2.42	-6.18	-3.76	FeS
FeS (ppt)	-2.27	-6.18	-3.92	FeS
Fluorite	-2.61	-13.38	-10.76	CaF2
Gypsum	-3.80	-8.39	-4.59	CaSO4:2H2O
H2 (g)	-8.18	-11.28	-3.09	H2
H2O (g)	-1.85	-0.00	1.85	H2O
H2S (g)	-3.96	-4.81	-0.85	H2S
Halite	-8.48	-6.93	1.55	NaCl
Hausmannite	-43.44	20.82	64.26	Mn3O4
Lepidocrocite	-6.85	9.85	16.70	FeOOH
Lime	-16.41	6.40	22.81	Ca (OH) 2
Mackinawite	-1.66	-6.18	-4.53	FeS
Magnetite	-20.35	25.45	45.80	Fe3O4
Manganite	-17.04	8.30	25.34	MnOOH
Marcasite	8.16	-9.94	-18.09	FeS2
Melanterite	-6.66	-9.04	-2.37	FeSO4:7H2O
Nesquehonite	-7.32	-12.76	-5.44	MgCO3:3H2O
O2 (g)	-71.14	-74.04	-2.90	O2
Pyrite	8.90	-9.94	-18.84	FeS2
Pyrochroite	-10.99	4.21	15.20	Mn (OH) 2
Pyrolusite	-31.07	12.40	43.47	MnO2
Rhodochrosite	-3.87	-14.95	-11.08	MnCO3
Siderite	-2.60	-13.41	-10.81	FeCO3
Sulfur	-1.82	3.37	5.19	S
Troilite	-0.06	-6.18	-6.12	FeS

End of simulation.

Reading input data for simulation 2.

SOLUTION 1 TS-MW01 3-18-2008 (Upgradient)

temp	13.6
pH	5.92
pe	4
redox	S (-2) / S (6)
units	mg/kgw
density	1
Cl	12
F	0.48
S (6)	3.5 as SO4
S (-2)	1.3


```

Ca          49
Fe (2)      2.32
Mg          22
Mn          0.59
K           9.2
Na          14
Alkalinity  365 as HCO3
water      1 # kg

```

END

Beginning of initial solution calculations.

Initial solution 1. TS-MW01 3-18-2008 (Upgradient)

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	5.982e-003	5.982e-003
Ca	1.223e-003	1.223e-003
Cl	3.385e-004	3.385e-004
F	2.527e-005	2.527e-005
Fe (2)	4.154e-005	4.154e-005
K	2.353e-004	2.353e-004
Mg	9.049e-004	9.049e-004
Mn	1.074e-005	1.074e-005
Na	6.090e-004	6.090e-004
S (-2)	4.054e-005	4.054e-005
S (6)	3.643e-005	3.643e-005

-----Description of solution-----

```

                                pH = 5.920
                                pe = 4.000
                    Activity of water = 1.000
                    Ionic strength = 7.792e-003
                    Mass of water (kg) = 1.000e+000
                    Total carbon (mol/kg) = 2.338e-002
                    Total CO2 (mol/kg) = 2.338e-002
                    Temperature (deg C) = 13.600
                    Electrical balance (eq) = -1.215e-003
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -10.67
                                Iterations = 11
                                Total H = 1.110185e+002
                                Total O = 5.555910e+001

```

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2)/S (6)	-2.1165	-0.1204

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.303e-006	1.202e-006	-5.885	-5.920	-0.035
OH-	3.650e-009	3.328e-009	-8.438	-8.478	-0.040
H2O	5.551e+001	9.995e-001	1.744	-0.000	0.000
C (4)	2.338e-002				
CO2	1.740e-002	1.743e-002	-1.759	-1.759	0.001
HCO3-	5.872e-003	5.378e-003	-2.231	-2.269	-0.038
CaHCO3+	4.931e-005	4.516e-005	-4.307	-4.345	-0.038
MgHCO3+	4.042e-005	3.692e-005	-4.393	-4.433	-0.039
FeHCO3+	1.213e-005	1.108e-005	-4.916	-4.955	-0.039
MnHCO3+	2.881e-006	2.631e-006	-5.540	-5.580	-0.039
NaHCO3	1.676e-006	1.679e-006	-5.776	-5.775	0.001
CO3-2	2.286e-007	1.608e-007	-6.641	-6.794	-0.153
CaCO3	1.858e-007	1.862e-007	-6.731	-6.730	0.001
FeCO3	7.932e-008	7.946e-008	-7.101	-7.100	0.001
MgCO3	7.823e-008	7.837e-008	-7.107	-7.106	0.001
MnCO3	6.998e-008	7.010e-008	-7.155	-7.154	0.001
NaCO3-	1.001e-009	9.140e-010	-9.000	-9.039	-0.039
Fe (CO3) (OH) -	2.814e-010	2.570e-010	-9.551	-9.590	-0.039
Fe (CO3) 2-2	2.158e-011	1.501e-011	-10.666	-10.824	-0.158
Ca	1.223e-003				
Ca+2	1.170e-003	8.223e-004	-2.932	-3.085	-0.153
CaHCO3+	4.931e-005	4.516e-005	-4.307	-4.345	-0.038
CaSO4	3.166e-006	3.172e-006	-5.500	-5.499	0.001
CaCO3	1.858e-007	1.862e-007	-6.731	-6.730	0.001
CaF+	1.318e-007	1.204e-007	-6.880	-6.919	-0.039
CaOH+	1.242e-010	1.135e-010	-9.906	-9.945	-0.039
CaHSO4+	2.157e-011	1.970e-011	-10.666	-10.706	-0.039
Cl	3.385e-004				
Cl-	3.385e-004	3.087e-004	-3.470	-3.510	-0.040
FeCl+	9.613e-009	8.779e-009	-8.017	-8.057	-0.039
MnCl+	7.558e-009	6.903e-009	-8.122	-8.161	-0.039
MnCl2	9.285e-013	9.301e-013	-12.032	-12.031	0.001
MnCl3-	8.659e-017	7.908e-017	-16.063	-16.102	-0.039
F	2.527e-005				
F-	2.430e-005	2.216e-005	-4.614	-4.654	-0.040
MgF+	7.870e-007	7.188e-007	-6.104	-6.143	-0.039
CaF+	1.318e-007	1.204e-007	-6.880	-6.919	-0.039
HF	3.264e-008	3.270e-008	-7.486	-7.485	0.001
NaF	7.065e-009	7.077e-009	-8.151	-8.150	0.001
FeF+	4.999e-009	4.565e-009	-8.301	-8.341	-0.039
MnF+	9.213e-010	8.414e-010	-9.036	-9.075	-0.039
HF2-	2.741e-012	2.503e-012	-11.562	-11.602	-0.039
Fe (2)	4.154e-005				
Fe+2	2.914e-005	2.060e-005	-4.536	-4.686	-0.151
FeHCO3+	1.213e-005	1.108e-005	-4.916	-4.955	-0.039
Fe (HS) 2	1.102e-007	1.104e-007	-6.958	-6.957	0.001
FeCO3	7.932e-008	7.946e-008	-7.101	-7.100	0.001
FeSO4	6.358e-008	6.370e-008	-7.197	-7.196	0.001
FeCl+	9.613e-009	8.779e-009	-8.017	-8.057	-0.039
FeF+	4.999e-009	4.565e-009	-8.301	-8.341	-0.039

FeOH+	2.446e-009	2.234e-009	-8.612	-8.651	-0.039
Fe (CO3) (OH) -	2.814e-010	2.570e-010	-9.551	-9.590	-0.039
Fe (HS) 3-	3.226e-011	2.947e-011	-10.491	-10.531	-0.039
Fe (CO3) 2-2	2.158e-011	1.501e-011	-10.666	-10.824	-0.158
FeHSO4+	5.403e-013	4.935e-013	-12.267	-12.307	-0.039
Fe (OH) 2	3.489e-014	3.496e-014	-13.457	-13.456	0.001
H (0)	3.931e-011				
H2	1.965e-011	1.969e-011	-10.707	-10.706	0.001
K	2.353e-004				
K+	2.353e-004	2.146e-004	-3.628	-3.668	-0.040
KSO4-	2.899e-008	2.647e-008	-7.538	-7.577	-0.039
KOH	6.174e-013	6.185e-013	-12.209	-12.209	0.001
Mg	9.049e-004				
Mg+2	8.613e-004	6.086e-004	-3.065	-3.216	-0.151
MgHCO3+	4.042e-005	3.692e-005	-4.393	-4.433	-0.039
MgSO4	2.266e-006	2.270e-006	-5.645	-5.644	0.001
MgF+	7.870e-007	7.188e-007	-6.104	-6.143	-0.039
MgCO3	7.823e-008	7.837e-008	-7.107	-7.106	0.001
MgOH+	2.976e-010	2.718e-010	-9.526	-9.566	-0.039
Mn (2)	1.074e-005				
Mn+2	7.763e-006	5.489e-006	-5.110	-5.261	-0.151
MnHCO3+	2.881e-006	2.631e-006	-5.540	-5.580	-0.039
MnCO3	6.998e-008	7.010e-008	-7.155	-7.154	0.001
MnSO4	1.678e-008	1.681e-008	-7.775	-7.774	0.001
MnCl+	7.558e-009	6.903e-009	-8.122	-8.161	-0.039
MnF+	9.213e-010	8.414e-010	-9.036	-9.075	-0.039
MnOH+	4.887e-011	4.464e-011	-10.311	-10.350	-0.039
MnCl2	9.285e-013	9.301e-013	-12.032	-12.031	0.001
MnCl3-	8.659e-017	7.908e-017	-16.063	-16.102	-0.039
Mn (3)	5.197e-034				
Mn+3	5.197e-034	2.297e-034	-33.284	-33.639	-0.355
Na	6.090e-004				
Na+	6.072e-004	5.551e-004	-3.217	-3.256	-0.039
NaHCO3	1.676e-006	1.679e-006	-5.776	-5.775	0.001
NaSO4-	6.101e-008	5.572e-008	-7.215	-7.254	-0.039
NaF	7.065e-009	7.077e-009	-8.151	-8.150	0.001
NaCO3-	1.001e-009	9.140e-010	-9.000	-9.039	-0.039
NaOH	3.043e-012	3.049e-012	-11.517	-11.516	0.001
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-74.795	-74.794	0.001
S (-2)	4.054e-005				
H2S	3.763e-005	3.770e-005	-4.424	-4.424	0.001
HS-	2.689e-006	2.452e-006	-5.570	-5.611	-0.040
Fe (HS) 2	1.102e-007	1.104e-007	-6.958	-6.957	0.001
Fe (HS) 3-	3.226e-011	2.947e-011	-10.491	-10.531	-0.039
S-2	1.560e-013	1.094e-013	-12.807	-12.961	-0.154
S (6)	3.643e-005				
SO4-2	3.083e-005	2.159e-005	-4.511	-4.666	-0.155
CaSO4	3.166e-006	3.172e-006	-5.500	-5.499	0.001
MgSO4	2.266e-006	2.270e-006	-5.645	-5.644	0.001
FeSO4	6.358e-008	6.370e-008	-7.197	-7.196	0.001
NaSO4-	6.101e-008	5.572e-008	-7.215	-7.254	-0.039
KSO4-	2.899e-008	2.647e-008	-7.538	-7.577	-0.039
MnSO4	1.678e-008	1.681e-008	-7.775	-7.774	0.001

HSO4-	2.181e-009	1.992e-009	-8.661	-8.701	-0.039
CaHSO4+	2.157e-011	1.970e-011	-10.666	-10.706	-0.039
FeHSO4+	5.403e-013	4.935e-013	-12.267	-12.307	-0.039

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH) 5]	-4.98	18.11	23.09	Fe2(OH) 5
[Fe3(OH) 7]	0.27	25.26	24.99	Fe3(OH) 7
[Fe3(OH) 8]	-13.05	29.07	42.12	Fe3(OH) 8
[Fe6(OH) 12] [CO3]	-26.46	31.89	58.35	Fe6(OH) 12 (CO3) 1
[Fe6(OH) 12] [SO4]	-26.36	34.02	60.38	Fe6(OH) 12 (SO4) 1
[Fe6(OH) 8] [Cl]	-20.57	22.99	43.56	Fe4(OH) 8 (Cl) 1
Anhydrite	-3.42	-7.75	-4.33	CaSO4
Aragonite	-1.61	-9.88	-8.27	CaCO3
Brucite	-8.17	8.62	16.79	Mg(OH) 2
Calcite	-1.45	-9.88	-8.42	CaCO3
CO2(g)	-0.44	-1.76	-1.32	CO2
Dolomite	-3.07	-19.89	-16.82	CaMg(CO3) 2
Epsomite	-5.66	-7.88	-2.22	MgSO4:7H2O
Fe(OH) 2 (1)	-5.79	7.15	12.94	Fe(OH) 2
Fe(OH) 2 (2)	-6.74	7.15	13.89	Fe(OH) 2
FeO	-6.44	7.15	13.59	FeO
FeS(am)	-0.60	-4.38	-3.78	FeS
FeS(ppt)	-0.46	-4.38	-3.92	FeS
Fluorite	-1.65	-12.39	-10.74	CaF2
Gypsum	-3.16	-7.75	-4.59	CaSO4:2H2O
H2(g)	-7.61	-10.71	-3.10	H2
H2O(g)	-1.82	-0.00	1.82	H2O
H2S(g)	-3.56	-4.42	-0.86	H2S
Halite	-8.32	-6.77	1.56	NaCl
Hausmannite	-36.62	27.34	63.96	Mn3O4
Lepidocrocite	-5.74	10.96	16.70	FeOOH
Lime	-14.06	8.75	22.81	Ca(OH) 2
Mackinawite	0.16	-4.38	-4.54	FeS
Magnetite	-16.73	29.07	45.80	Fe3O4
Manganite	-14.96	10.38	25.34	MnOOH
Marcasite	9.76	-8.30	-18.06	FeS2
Melanterite	-7.00	-9.35	-2.36	FeSO4:7H2O
Nesquehonite	-4.56	-10.01	-5.45	MgCO3:3H2O
O2(g)	-71.89	-74.79	-2.91	O2
Pyrite	10.51	-8.30	-18.81	FeS2
Pyrochroite	-8.62	6.58	15.20	Mn(OH) 2
Pyrolusite	-29.09	14.19	43.28	MnO2
Rhodochrosite	-0.97	-12.05	-11.09	MnCO3
Siderite	-0.66	-11.48	-10.82	FeCO3
Sulfur	-1.98	3.18	5.16	S
Troilite	1.75	-4.38	-6.13	FeS

End of simulation.

Reading input data for simulation 3.

SOLUTION 1 TS-MW02 3-19-2008 (Between Walls)

temp 14.2
pH 5.58
pe 4
redox S(-2)/S(6)
units mg/kgw
density 1
Cl 9.7
F 0.44
S(6) 15 as SO4
S(-2) 1.0
Ca 14
Fe(2) 1.95
Mg 8.1
Mn 0.098
K 2.4
Na 15
Alkalinity 84 as CaCO3
water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. TS-MW02 3-19-2008 (Between Walls)

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.678e-003	1.678e-003
Ca	3.493e-004	3.493e-004
Cl	2.736e-004	2.736e-004
F	2.316e-005	2.316e-005
Fe(2)	3.492e-005	3.492e-005
K	6.138e-005	6.138e-005
Mg	3.332e-004	3.332e-004
Mn	1.784e-006	1.784e-006
Na	6.525e-004	6.525e-004
S(-2)	3.119e-005	3.119e-005
S(6)	1.561e-004	1.561e-004

-----Description of solution-----

pH = 5.580
pe = 4.000
Activity of water = 1.000
Ionic strength = 3.024e-003

Mass of water (kg) = 1.000e+000
 Total carbon (mol/kg) = 1.269e-002
 Total CO2 (mol/kg) = 1.269e-002
 Temperature (deg C) = 14.200
 Electrical balance (eq) = -1.353e-004
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -3.10
 Iterations = 11
 Total H = 1.110142e+002
 Total O = 5.553390e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-1.6020	-0.0913

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.778e-006	2.630e-006	-5.556	-5.580	-0.024
OH-	1.700e-009	1.601e-009	-8.770	-8.796	-0.026
H2O	5.551e+001	9.998e-001	1.744	-0.000	0.000
C(4)	1.269e-002				
CO2	1.101e-002	1.102e-002	-1.958	-1.958	0.000
HCO3-	1.666e-003	1.572e-003	-2.778	-2.803	-0.025
MgHCO3+	4.836e-006	4.558e-006	-5.316	-5.341	-0.026
CaHCO3+	4.643e-006	4.382e-006	-5.333	-5.358	-0.025
FeHCO3+	4.038e-006	3.806e-006	-5.394	-5.420	-0.026
NaHCO3	5.430e-007	5.433e-007	-6.265	-6.265	0.000
MnHCO3+	1.861e-007	1.754e-007	-6.730	-6.756	-0.026
CO3-2	2.751e-008	2.183e-008	-7.561	-7.661	-0.100
FeCO3	1.267e-008	1.268e-008	-7.897	-7.897	0.000
CaCO3	8.317e-009	8.323e-009	-8.080	-8.080	0.000
MgCO3	4.527e-009	4.530e-009	-8.344	-8.344	0.000
MnCO3	2.169e-009	2.170e-009	-8.664	-8.663	0.000
NaCO3-	1.506e-010	1.419e-010	-9.822	-9.848	-0.026
Fe(CO3)(OH)-	1.989e-011	1.875e-011	-10.701	-10.727	-0.026
Fe(CO3)2-2	4.118e-013	3.252e-013	-12.385	-12.488	-0.103
Ca	3.493e-004				
Ca+2	3.391e-004	2.690e-004	-3.470	-3.570	-0.101
CaSO4	5.534e-006	5.538e-006	-5.257	-5.257	0.000
CaHCO3+	4.643e-006	4.382e-006	-5.333	-5.358	-0.025
CaF+	4.097e-008	3.862e-008	-7.388	-7.413	-0.026
CaCO3	8.317e-009	8.323e-009	-8.080	-8.080	0.000
CaHSO4+	8.028e-011	7.568e-011	-10.095	-10.121	-0.026
CaOH+	1.800e-011	1.697e-011	-10.745	-10.770	-0.026
Cl	2.736e-004				
Cl-	2.736e-004	2.578e-004	-3.563	-3.589	-0.026
FeCl+	9.137e-009	8.613e-009	-8.039	-8.065	-0.026
MnCl+	1.394e-009	1.314e-009	-8.856	-8.881	-0.026
MnCl2	1.478e-013	1.479e-013	-12.830	-12.830	0.000
MnCl3-	1.114e-017	1.050e-017	-16.953	-16.979	-0.026

F	2.316e-005					
F-	2.272e-005	2.141e-005	-4.644	-4.669	-0.026	
MgF+	3.144e-007	2.963e-007	-6.503	-6.528	-0.026	
HF	6.979e-008	6.983e-008	-7.156	-7.156	0.000	
CaF+	4.097e-008	3.862e-008	-7.388	-7.413	-0.026	
NaF	7.564e-009	7.569e-009	-8.121	-8.121	0.000	
FeF+	5.497e-009	5.182e-009	-8.260	-8.286	-0.026	
MnF+	1.966e-010	1.853e-010	-9.706	-9.732	-0.026	
HF2-	5.513e-012	5.197e-012	-11.259	-11.284	-0.026	
Fe (2)	3.492e-005					
Fe+2	3.043e-005	2.421e-005	-4.517	-4.616	-0.099	
FeHCO3+	4.038e-006	3.806e-006	-5.394	-5.420	-0.026	
FeSO4	4.015e-007	4.018e-007	-6.396	-6.396	0.000	
Fe (HS) 2	1.815e-008	1.816e-008	-7.741	-7.741	0.000	
FeCO3	1.267e-008	1.268e-008	-7.897	-7.897	0.000	
FeCl+	9.137e-009	8.613e-009	-8.039	-8.065	-0.026	
FeF+	5.497e-009	5.182e-009	-8.260	-8.286	-0.026	
FeOH+	1.336e-009	1.259e-009	-8.874	-8.900	-0.026	
Fe (CO3) (OH) -	1.989e-011	1.875e-011	-10.701	-10.727	-0.026	
FeHSO4+	7.224e-012	6.810e-012	-11.141	-11.167	-0.026	
Fe (HS) 3-	1.925e-012	1.815e-012	-11.716	-11.741	-0.026	
Fe (CO3) 2-2	4.118e-013	3.252e-013	-12.385	-12.488	-0.103	
Fe (OH) 2	8.578e-015	8.584e-015	-14.067	-14.066	0.000	
H (0)	1.751e-011					
H2	8.755e-012	8.761e-012	-11.058	-11.057	0.000	
K	6.138e-005					
K+	6.134e-005	5.779e-005	-4.212	-4.238	-0.026	
KSO4-	4.059e-008	3.826e-008	-7.392	-7.417	-0.026	
KOH	7.611e-014	7.617e-014	-13.119	-13.118	0.000	
Mg	3.332e-004					
Mg+2	3.229e-004	2.567e-004	-3.491	-3.591	-0.100	
MgSO4	5.162e-006	5.165e-006	-5.287	-5.287	0.000	
MgHCO3+	4.836e-006	4.558e-006	-5.316	-5.341	-0.026	
MgF+	3.144e-007	2.963e-007	-6.503	-6.528	-0.026	
MgCO3	4.527e-009	4.530e-009	-8.344	-8.344	0.000	
MgOH+	5.895e-011	5.557e-011	-10.230	-10.255	-0.026	
Mn (2)	1.784e-006					
Mn+2	1.573e-006	1.252e-006	-5.803	-5.903	-0.099	
MnHCO3+	1.861e-007	1.754e-007	-6.730	-6.756	-0.026	
MnSO4	2.058e-008	2.059e-008	-7.687	-7.686	0.000	
MnCO3	2.169e-009	2.170e-009	-8.664	-8.663	0.000	
MnCl+	1.394e-009	1.314e-009	-8.856	-8.881	-0.026	
MnF+	1.966e-010	1.853e-010	-9.706	-9.732	-0.026	
MnOH+	5.203e-012	4.905e-012	-11.284	-11.309	-0.026	
MnCl2	1.478e-013	1.479e-013	-12.830	-12.830	0.000	
MnCl3-	1.114e-017	1.050e-017	-16.953	-16.979	-0.026	
Mn (3)	3.202e-034					
Mn+3	3.202e-034	1.882e-034	-33.495	-33.725	-0.231	
Na	6.525e-004					
Na+	6.516e-004	6.145e-004	-3.186	-3.211	-0.025	
NaHCO3	5.430e-007	5.433e-007	-6.265	-6.265	0.000	
NaSO4-	3.486e-007	3.286e-007	-6.458	-6.483	-0.026	
NaF	7.564e-009	7.569e-009	-8.121	-8.121	0.000	
NaCO3-	1.506e-010	1.419e-010	-9.822	-9.848	-0.026	

NaOH	1.542e-012	1.543e-012	-11.812	-11.812	0.000
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-73.882	-73.882	0.000
S(-2)	3.119e-005				
H2S	3.018e-005	3.020e-005	-4.520	-4.520	0.000
HS-	9.740e-007	9.176e-007	-6.011	-6.037	-0.026
Fe(HS)2	1.815e-008	1.816e-008	-7.741	-7.741	0.000
Fe(HS)3-	1.925e-012	1.815e-012	-11.716	-11.741	-0.026
S-2	2.468e-014	1.956e-014	-13.608	-13.709	-0.101
S(6)	1.561e-004				
SO4-2	1.446e-004	1.146e-004	-3.840	-3.941	-0.101
CaSO4	5.534e-006	5.538e-006	-5.257	-5.257	0.000
MgSO4	5.162e-006	5.165e-006	-5.287	-5.287	0.000
FeSO4	4.015e-007	4.018e-007	-6.396	-6.396	0.000
NaSO4-	3.486e-007	3.286e-007	-6.458	-6.483	-0.026
KSO4-	4.059e-008	3.826e-008	-7.392	-7.417	-0.026
HSO4-	2.482e-008	2.340e-008	-7.605	-7.631	-0.026
MnSO4	2.058e-008	2.059e-008	-7.687	-7.686	0.000
CaHSO4+	8.028e-011	7.568e-011	-10.095	-10.121	-0.026
FeHSO4+	7.224e-012	6.810e-012	-11.141	-11.167	-0.026

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH)5]	-6.02	17.07	23.09	Fe2(OH)5
[Fe3(OH)7]	-1.38	23.61	24.99	Fe3(OH)7
[Fe3(OH)8]	-14.53	27.59	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-29.95	28.40	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-28.26	32.12	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-22.58	20.98	43.56	Fe4(OH)8(Cl)1
Anhydrite	-3.18	-7.51	-4.33	CaSO4
Aragonite	-2.96	-11.23	-8.27	CaCO3
Brucite	-9.22	7.57	16.79	Mg(OH)2
Calcite	-2.80	-11.23	-8.43	CaCO3
CO2(g)	-0.63	-1.96	-1.33	CO2
Dolomite	-5.65	-22.48	-16.83	CaMg(CO3)2
Epsomite	-5.31	-7.53	-2.22	MgSO4:7H2O
Fe(OH)2(1)	-6.40	6.54	12.94	Fe(OH)2
Fe(OH)2(2)	-7.35	6.54	13.89	Fe(OH)2
FeO	-7.05	6.54	13.59	FeO
FeS(am)	-1.29	-5.07	-3.78	FeS
FeS(ppt)	-1.16	-5.07	-3.92	FeS
Fluorite	-2.17	-12.91	-10.74	CaF2
Gypsum	-2.93	-7.51	-4.59	CaSO4:2H2O
H2(g)	-7.96	-11.06	-3.10	H2
H2O(g)	-1.80	-0.00	1.80	H2O
H2S(g)	-3.65	-4.52	-0.87	H2S
Halite	-8.36	-6.80	1.56	NaCl
Hausmannite	-40.07	23.73	63.80	Mn3O4
Lepidocrocite	-6.18	10.52	16.70	FeOOH
Lime	-15.22	7.59	22.81	Ca(OH)2
Mackinawite	-0.53	-5.07	-4.54	FeS
Magnetite	-18.21	27.59	45.80	Fe3O4

Manganite	-16.10	9.24	25.34	MnOOH
Marcasite	9.31	-8.73	-18.05	FeS2
Melanterite	-6.21	-8.56	-2.35	FeSO4:7H2O
Nesquehonite	-5.79	-11.25	-5.46	MgCO3:3H2O
O2(g)	-70.97	-73.88	-2.91	O2
Pyrite	10.06	-8.73	-18.79	FeS2
Pyrochroite	-9.94	5.26	15.20	Mn(OH)2
Pyrolusite	-29.96	13.21	43.17	MnO2
Rhodochrosite	-2.47	-13.56	-11.09	MnCO3
Siderite	-1.46	-12.28	-10.82	FeCO3
Sulfur	-1.71	3.44	5.14	S
Troilite	1.06	-5.07	-6.13	FeS

End of simulation.

Reading input data for simulation 4.

SOLUTION 1 TS-MW03 3-19-2008 (In downgradient wall)

temp	13.9
pH	6.17
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	12
F	0.47
S(6)	7.5 as SO4
S(-2)	1.6
Ca	120
Fe(2)	1.9
Mg	30
Mn	0.59
K	19
Na	14
Alkalinity	647 as HCO3
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. TS-MW03 3-19-2008 (In downgradient wall)

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.060e-002	1.060e-002
Ca	2.994e-003	2.994e-003
Cl	3.385e-004	3.385e-004

F	2.474e-005	2.474e-005
Fe (2)	3.402e-005	3.402e-005
K	4.859e-004	4.859e-004
Mg	1.234e-003	1.234e-003
Mn	1.074e-005	1.074e-005
Na	6.090e-004	6.090e-004
S (-2)	4.990e-005	4.990e-005
S (6)	7.807e-005	7.807e-005

-----Description of solution-----

pH	=	6.170
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	1.407e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	2.721e-002
Total CO2 (mol/kg)	=	2.721e-002
Temperature (deg C)	=	13.900
Electrical balance (eq)	=	-1.482e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	-7.38
Iterations	=	11
Total H	=	1.110231e+002
Total O	=	5.557154e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2)/S (6)	-2.4123	-0.1374

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	7.482e-007	6.761e-007	-6.126	-6.170	-0.044
OH-	6.847e-009	6.071e-009	-8.164	-8.217	-0.052
H2O	5.551e+001	9.994e-001	1.744	-0.000	0.000
C (4)	2.721e-002				
CO2	1.661e-002	1.667e-002	-1.780	-1.778	0.001
HCO3-	1.030e-002	9.198e-003	-1.987	-2.036	-0.049
CaHCO3+	1.881e-004	1.680e-004	-3.726	-3.775	-0.049
MgHCO3+	8.553e-005	7.606e-005	-4.068	-4.119	-0.051
FeHCO3+	1.336e-005	1.188e-005	-4.874	-4.925	-0.051
MnHCO3+	3.919e-006	3.485e-006	-5.407	-5.458	-0.051
NaHCO3	2.783e-006	2.792e-006	-5.556	-5.554	0.001
CaCO3	1.232e-006	1.236e-006	-5.909	-5.908	0.001
CO3-2	7.747e-007	4.929e-007	-6.111	-6.307	-0.196
MgCO3	2.897e-007	2.906e-007	-6.538	-6.537	0.001
MnCO3	1.659e-007	1.665e-007	-6.780	-6.779	0.001
FeCO3	1.522e-007	1.527e-007	-6.817	-6.816	0.001
NaCO3-	3.114e-009	2.770e-009	-8.507	-8.558	-0.051
Fe (CO3) (OH) -	9.877e-010	8.783e-010	-9.005	-9.056	-0.051

	Fe (CO ₃) ²⁻	1.414e-010	8.845e-011	-9.850	-10.053	-0.204
Ca		2.994e-003				
	Ca ²⁺	2.792e-003	1.776e-003	-2.554	-2.751	-0.197
	CaHCO ₃ ⁺	1.881e-004	1.680e-004	-3.726	-3.775	-0.049
	CaSO ₄	1.216e-005	1.220e-005	-4.915	-4.914	0.001
	CaCO ₃	1.232e-006	1.236e-006	-5.909	-5.908	0.001
	CaF ⁺	2.771e-007	2.464e-007	-6.557	-6.608	-0.051
	CaOH ⁺	4.899e-010	4.357e-010	-9.310	-9.361	-0.051
	CaHSO ₄ ⁺	4.806e-011	4.274e-011	-10.318	-10.369	-0.051
Cl		3.385e-004				
	Cl ⁻	3.385e-004	3.002e-004	-3.470	-3.523	-0.052
	FeCl ⁺	6.019e-009	5.353e-009	-8.220	-8.271	-0.051
	MnCl ⁺	5.847e-009	5.200e-009	-8.233	-8.284	-0.051
	MnCl ₂	6.793e-013	6.815e-013	-12.168	-12.167	0.001
	MnCl ₃ ⁻	6.337e-017	5.635e-017	-16.198	-16.249	-0.051
F		2.474e-005				
	F ⁻	2.351e-005	2.085e-005	-4.629	-4.681	-0.052
	MgF ⁺	9.209e-007	8.189e-007	-6.036	-6.087	-0.051
	CaF ⁺	2.771e-007	2.464e-007	-6.557	-6.608	-0.051
	HF	1.734e-008	1.739e-008	-7.761	-7.760	0.001
	NaF	6.454e-009	6.475e-009	-8.190	-8.189	0.001
	FeF ⁺	3.028e-009	2.693e-009	-8.519	-8.570	-0.051
	MnF ⁺	6.895e-010	6.132e-010	-9.161	-9.212	-0.051
	HF ₂ ⁻	1.413e-012	1.256e-012	-11.850	-11.901	-0.051
Fe (2)		3.402e-005				
	Fe ²⁺	2.013e-005	1.292e-005	-4.696	-4.889	-0.193
	FeHCO ₃ ⁺	1.336e-005	1.188e-005	-4.874	-4.925	-0.051
	Fe (HS) ²⁻	2.993e-007	3.003e-007	-6.524	-6.522	0.001
	FeCO ₃	1.522e-007	1.527e-007	-6.817	-6.816	0.001
	FeSO ₄	7.113e-008	7.136e-008	-7.148	-7.147	0.001
	FeCl ⁺	6.019e-009	5.353e-009	-8.220	-8.271	-0.051
	FeF ⁺	3.028e-009	2.693e-009	-8.519	-8.570	-0.051
	FeOH ⁺	2.869e-009	2.551e-009	-8.542	-8.593	-0.051
	Fe (CO ₃) (OH) ⁻	9.877e-010	8.783e-010	-9.005	-9.056	-0.051
	Fe (HS) ³⁻	1.878e-010	1.670e-010	-9.726	-9.777	-0.051
	Fe (CO ₃) ²⁻	1.414e-010	8.845e-011	-9.850	-10.053	-0.204
	FeHSO ₄ ⁺	3.496e-013	3.109e-013	-12.456	-12.507	-0.051
	Fe (OH) ²⁻	6.906e-014	6.929e-014	-13.161	-13.159	0.001
H (0)		4.832e-011				
	H ₂	2.416e-011	2.424e-011	-10.617	-10.615	0.001
K		4.859e-004				
	K ⁺	4.858e-004	4.309e-004	-3.314	-3.366	-0.052
	KSO ₄ ⁻	1.068e-007	9.498e-008	-6.971	-7.022	-0.051
	KOH	2.202e-012	2.209e-012	-11.657	-11.656	0.001
Mg		1.234e-003				
	Mg ²⁺	1.142e-003	7.327e-004	-2.942	-3.135	-0.193
	MgHCO ₃ ⁺	8.553e-005	7.606e-005	-4.068	-4.119	-0.051
	MgSO ₄	4.880e-006	4.896e-006	-5.312	-5.310	0.001
	MgF ⁺	9.209e-007	8.189e-007	-6.036	-6.087	-0.051
	MgCO ₃	2.897e-007	2.906e-007	-6.538	-6.537	0.001
	MgOH ⁺	6.737e-010	5.991e-010	-9.172	-9.222	-0.051
Mn (2)		1.074e-005				
	Mn ²⁺	6.625e-006	4.251e-006	-5.179	-5.371	-0.193
	MnHCO ₃ ⁺	3.919e-006	3.485e-006	-5.407	-5.458	-0.051

MnCO3	1.659e-007	1.665e-007	-6.780	-6.779	0.001
MnSO4	2.320e-008	2.327e-008	-7.635	-7.633	0.001
MnCl+	5.847e-009	5.200e-009	-8.233	-8.284	-0.051
MnF+	6.895e-010	6.132e-010	-9.161	-9.212	-0.051
MnOH+	7.097e-011	6.312e-011	-10.149	-10.200	-0.051
MnCl2	6.793e-013	6.815e-013	-12.168	-12.167	0.001
MnCl3-	6.337e-017	5.635e-017	-16.198	-16.249	-0.051
Mn (3)	2.713e-034				
Mn+3	2.713e-034	9.439e-035	-33.567	-34.025	-0.459
Na	6.090e-004				
Na+	6.061e-004	5.397e-004	-3.217	-3.268	-0.050
NaHCO3	2.783e-006	2.792e-006	-5.556	-5.554	0.001
NaSO4-	1.085e-007	9.645e-008	-6.965	-7.016	-0.051
NaF	6.454e-009	6.475e-009	-8.190	-8.189	0.001
NaCO3-	3.114e-009	2.770e-009	-8.507	-8.558	-0.051
NaOH	5.255e-012	5.272e-012	-11.279	-11.278	0.001
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-74.872	-74.870	0.001
S (-2)	4.990e-005				
H2S	4.354e-005	4.368e-005	-4.361	-4.360	0.001
HS-	5.760e-006	5.107e-006	-5.240	-5.292	-0.052
Fe (HS) 2	2.993e-007	3.003e-007	-6.524	-6.522	0.001
Fe (HS) 3-	1.878e-010	1.670e-010	-9.726	-9.777	-0.051
S-2	6.548e-013	4.142e-013	-12.184	-12.383	-0.199
S (6)	7.807e-005				
SO4-2	6.072e-005	3.836e-005	-4.217	-4.416	-0.199
CaSO4	1.216e-005	1.220e-005	-4.915	-4.914	0.001
MgSO4	4.880e-006	4.896e-006	-5.312	-5.310	0.001
NaSO4-	1.085e-007	9.645e-008	-6.965	-7.016	-0.051
KSO4-	1.068e-007	9.498e-008	-6.971	-7.022	-0.051
FeSO4	7.113e-008	7.136e-008	-7.148	-7.147	0.001
MnSO4	2.320e-008	2.327e-008	-7.635	-7.633	0.001
HSO4-	2.251e-009	2.002e-009	-8.648	-8.699	-0.051
CaHSO4+	4.806e-011	4.274e-011	-10.318	-10.369	-0.051
FeHSO4+	3.496e-013	3.109e-013	-12.456	-12.507	-0.051

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-4.43	18.66	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	1.12	26.11	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-12.25	29.87	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-24.78	33.57	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-24.92	35.46	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-19.69	23.87	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-2.83	-7.17	-4.33	CaSO4
Aragonite	-0.78	-9.06	-8.27	CaCO3
Brucite	-7.59	9.20	16.79	Mg (OH) 2
Calcite	-0.63	-9.06	-8.43	CaCO3
CO2 (g)	-0.45	-1.78	-1.33	CO2
Dolomite	-1.68	-18.50	-16.82	CaMg (CO3) 2
Epsomite	-5.33	-7.55	-2.22	MgSO4:7H2O
Fe (OH) 2 (1)	-5.49	7.45	12.94	Fe (OH) 2

Fe (OH) 2 (2)	-6.44	7.45	13.89	Fe (OH) 2
FeO	-6.14	7.45	13.59	FeO
FeS (am)	-0.23	-4.01	-3.78	FeS
FeS (ppt)	-0.10	-4.01	-3.92	FeS
Fluorite	-1.37	-12.11	-10.74	CaF2
Gypsum	-2.58	-7.17	-4.59	CaSO4:2H2O
H2 (g)	-7.52	-10.62	-3.10	H2
H2O (g)	-1.81	-0.00	1.81	H2O
H2S (g)	-3.49	-4.36	-0.87	H2S
Halite	-8.35	-6.79	1.56	NaCl
Hausmannite	-35.46	28.42	63.88	Mn3O4
Lepidocrocite	-5.49	11.21	16.70	FeOOH
Lime	-13.22	9.59	22.81	Ca (OH) 2
Mackinawite	0.53	-4.01	-4.54	FeS
Magnetite	-15.93	29.87	45.80	Fe3O4
Manganite	-14.61	10.73	25.34	MnOOH
Marcasite	10.10	-7.96	-18.06	FeS2
Melanterite	-6.95	-9.31	-2.35	FeSO4:7H2O
Nesquehonite	-3.99	-9.44	-5.46	MgCO3:3H2O
O2 (g)	-71.96	-74.87	-2.91	O2
Pyrite	10.84	-7.96	-18.80	FeS2
Pyrochroite	-8.23	6.97	15.20	Mn (OH) 2
Pyrolusite	-28.74	14.48	43.23	MnO2
Rhodochrosite	-0.59	-11.68	-11.09	MnCO3
Siderite	-0.38	-11.20	-10.82	FeCO3
Sulfur	-2.00	3.16	5.15	S
Troilite	2.12	-4.01	-6.13	FeS

End of simulation.

Reading input data for simulation 5.

SOLUTION 1 TS-MW04 3-19-2008 (15 ft downgradient)

temp	13.3
pH	5.59
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	9.8
F	0.44
S(6)	9.2 as SO4
S(-2)	1.0
Ca	10
Fe(2)	0.005
Mg	6.4
Mn	0.14
K	1.0
Na	12
Alkalinity	70 as CaCO3

water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. TS-MW04 3-19-2008 (15 ft downgradient)

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.399e-003	1.399e-003
Ca	2.495e-004	2.495e-004
Cl	2.764e-004	2.764e-004
F	2.316e-005	2.316e-005
Fe(2)	8.953e-008	8.953e-008
K	2.557e-005	2.557e-005
Mg	2.632e-004	2.632e-004
Mn	2.548e-006	2.548e-006
Na	5.220e-004	5.220e-004
S(-2)	3.119e-005	3.119e-005
S(6)	9.577e-005	9.577e-005

-----Description of solution-----

pH	=	5.590
pe	=	4.000
Activity of water	=	1.000
Ionic strength	=	2.313e-003
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	1.062e-002
Total CO2 (mol/kg)	=	1.062e-002
Temperature (deg C)	=	13.300
Electrical balance (eq)	=	-3.115e-004
Percent error, 100*(Cat- An)/(Cat+ An)	=	-9.06
Iterations	=	10
Total H	=	1.110139e+002
Total O	=	5.552925e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-1.6190	-0.0920

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.698e-006	2.570e-006	-5.569	-5.590	-0.021

OH-	1.599e-009	1.518e-009	-8.796	-8.819	-0.023
H2O	5.551e+001	9.998e-001	1.744	-0.000	0.000
C (4)	1.062e-002				
CO2	9.224e-003	9.229e-003	-2.035	-2.035	0.000
HCO3-	1.394e-003	1.324e-003	-2.856	-2.878	-0.022
MgHCO3+	3.301e-006	3.134e-006	-5.481	-5.504	-0.023
CaHCO3+	2.810e-006	2.671e-006	-5.551	-5.573	-0.022
NaHCO3	3.686e-007	3.688e-007	-6.433	-6.433	0.000
MnHCO3+	2.327e-007	2.209e-007	-6.633	-6.656	-0.023
CO3-2	2.253e-008	1.837e-008	-7.647	-7.736	-0.089
FeHCO3+	9.077e-009	8.617e-009	-8.042	-8.065	-0.023
CaCO3	5.128e-009	5.131e-009	-8.290	-8.290	0.000
MgCO3	3.072e-009	3.074e-009	-8.513	-8.512	0.000
MnCO3	2.729e-009	2.731e-009	-8.564	-8.564	0.000
NaCO3-	9.654e-011	9.165e-011	-10.015	-10.038	-0.023
FeCO3	2.866e-011	2.867e-011	-10.543	-10.543	0.000
Fe (CO3) (OH) -	4.571e-014	4.339e-014	-13.340	-13.363	-0.023
Fe (CO3) 2-2	7.620e-016	6.189e-016	-15.118	-15.208	-0.090
Ca	2.495e-004				
Ca+2	2.441e-004	1.989e-004	-3.613	-3.701	-0.089
CaHCO3+	2.810e-006	2.671e-006	-5.551	-5.573	-0.022
CaSO4	2.603e-006	2.605e-006	-5.584	-5.584	0.000
CaF+	2.973e-008	2.822e-008	-7.527	-7.549	-0.023
CaCO3	5.128e-009	5.131e-009	-8.290	-8.290	0.000
CaHSO4+	3.632e-011	3.448e-011	-10.440	-10.462	-0.023
CaOH+	1.353e-011	1.284e-011	-10.869	-10.891	-0.023
Cl	2.764e-004				
Cl-	2.764e-004	2.623e-004	-3.558	-3.581	-0.023
MnCl+	2.107e-009	2.000e-009	-8.676	-8.699	-0.023
FeCl+	2.482e-011	2.356e-011	-10.605	-10.628	-0.023
MnCl2	2.289e-013	2.290e-013	-12.640	-12.640	0.000
MnCl3-	1.743e-017	1.654e-017	-16.759	-16.781	-0.023
F	2.316e-005				
F-	2.280e-005	2.164e-005	-4.642	-4.665	-0.023
MgF+	2.535e-007	2.406e-007	-6.596	-6.619	-0.023
HF	6.789e-008	6.792e-008	-7.168	-7.168	0.000
CaF+	2.973e-008	2.822e-008	-7.527	-7.549	-0.023
NaF	6.162e-009	6.165e-009	-8.210	-8.210	0.000
MnF+	2.951e-010	2.801e-010	-9.530	-9.553	-0.023
FeF+	1.483e-011	1.408e-011	-10.829	-10.851	-0.023
HF2-	5.330e-012	5.060e-012	-11.273	-11.296	-0.023
Fe (2)	8.953e-008				
Fe+2	7.965e-008	6.506e-008	-7.099	-7.187	-0.088
FeHCO3+	9.077e-009	8.617e-009	-8.042	-8.065	-0.023
FeSO4	6.805e-010	6.808e-010	-9.167	-9.167	0.000
Fe (HS) 2	4.797e-011	4.799e-011	-10.319	-10.319	0.000
FeCO3	2.866e-011	2.867e-011	-10.543	-10.543	0.000
FeCl+	2.482e-011	2.356e-011	-10.605	-10.628	-0.023
FeF+	1.483e-011	1.408e-011	-10.829	-10.851	-0.023
FeOH+	3.393e-012	3.221e-012	-11.469	-11.492	-0.023
Fe (CO3) (OH) -	4.571e-014	4.339e-014	-13.340	-13.363	-0.023
FeHSO4+	1.188e-014	1.128e-014	-13.925	-13.948	-0.023
Fe (HS) 3-	5.008e-015	4.755e-015	-14.300	-14.323	-0.023
Fe (CO3) 2-2	7.620e-016	6.189e-016	-15.118	-15.208	-0.090

Fe (OH) 2	2.415e-017	2.416e-017	-16.617	-16.617	0.000
H (0)	1.825e-011				
H2	9.127e-012	9.132e-012	-11.040	-11.039	0.000
K	2.557e-005				
K+	2.556e-005	2.426e-005	-4.592	-4.615	-0.023
KSO4-	1.067e-008	1.013e-008	-7.972	-7.994	-0.023
KOH	3.270e-014	3.272e-014	-13.485	-13.485	0.000
Mg	2.632e-004				
Mg+2	2.570e-004	2.099e-004	-3.590	-3.678	-0.088
MgHCO3+	3.301e-006	3.134e-006	-5.481	-5.504	-0.023
MgSO4	2.642e-006	2.643e-006	-5.578	-5.578	0.000
MgF+	2.535e-007	2.406e-007	-6.596	-6.619	-0.023
MgCO3	3.072e-009	3.074e-009	-8.513	-8.512	0.000
MgOH+	4.486e-011	4.259e-011	-10.348	-10.371	-0.023
Mn (2)	2.548e-006				
Mn+2	2.291e-006	1.871e-006	-5.640	-5.728	-0.088
MnHCO3+	2.327e-007	2.209e-007	-6.633	-6.656	-0.023
MnSO4	1.939e-008	1.940e-008	-7.713	-7.712	0.000
MnCO3	2.729e-009	2.731e-009	-8.564	-8.564	0.000
MnCl+	2.107e-009	2.000e-009	-8.676	-8.699	-0.023
MnF+	2.951e-010	2.801e-010	-9.530	-9.553	-0.023
MnOH+	7.304e-012	6.934e-012	-11.136	-11.159	-0.023
MnCl2	2.289e-013	2.290e-013	-12.640	-12.640	0.000
MnCl3-	1.743e-017	1.654e-017	-16.759	-16.781	-0.023
Mn (3)	3.751e-034				
Mn+3	3.751e-034	2.349e-034	-33.426	-33.629	-0.203
Na	5.220e-004				
Na+	5.214e-004	4.952e-004	-3.283	-3.305	-0.022
NaHCO3	3.686e-007	3.688e-007	-6.433	-6.433	0.000
NaSO4-	1.779e-007	1.689e-007	-6.750	-6.772	-0.023
NaF	6.162e-009	6.165e-009	-8.210	-8.210	0.000
NaCO3-	9.654e-011	9.165e-011	-10.015	-10.038	-0.023
NaOH	1.272e-012	1.272e-012	-11.896	-11.895	0.000
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-74.232	-74.231	0.000
S (-2)	3.119e-005				
H2S	3.023e-005	3.024e-005	-4.520	-4.519	0.000
HS-	9.588e-007	9.098e-007	-6.018	-6.041	-0.023
Fe (HS) 2	4.797e-011	4.799e-011	-10.319	-10.319	0.000
S-2	2.279e-014	1.856e-014	-13.642	-13.731	-0.089
Fe (HS) 3-	5.008e-015	4.755e-015	-14.300	-14.323	-0.023
S (6)	9.577e-005				
SO4-2	9.030e-005	7.352e-005	-4.044	-4.134	-0.089
MgSO4	2.642e-006	2.643e-006	-5.578	-5.578	0.000
CaSO4	2.603e-006	2.605e-006	-5.584	-5.584	0.000
NaSO4-	1.779e-007	1.689e-007	-6.750	-6.772	-0.023
MnSO4	1.939e-008	1.940e-008	-7.713	-7.712	0.000
HSO4-	1.519e-008	1.442e-008	-7.819	-7.841	-0.023
KSO4-	1.067e-008	1.013e-008	-7.972	-7.994	-0.023
FeSO4	6.805e-010	6.808e-010	-9.167	-9.167	0.000
CaHSO4+	3.632e-011	3.448e-011	-10.440	-10.462	-0.023
FeHSO4+	1.188e-014	1.128e-014	-13.925	-13.948	-0.023

-----Saturation indices-----

Phase	SI log IAP		log KT	
[Fe2(OH)5]	-11.13	11.96	23.09	Fe2(OH)5
[Fe3(OH)7]	-9.04	15.95	24.99	Fe3(OH)7
[Fe3(OH)8]	-22.20	19.92	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-45.36	12.99	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-43.79	16.59	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-32.79	10.77	43.56	Fe4(OH)8(Cl)1
Anhydrite	-3.50	-7.83	-4.33	CaSO4
Aragonite	-3.17	-11.44	-8.27	CaCO3
Brucite	-9.29	7.50	16.79	Mg(OH)2
Calcite	-3.01	-11.44	-8.42	CaCO3
CO2(g)	-0.72	-2.03	-1.32	CO2
Dolomite	-6.04	-22.85	-16.81	CaMg(CO3)2
Epsomite	-5.59	-7.81	-2.22	MgSO4·7H2O
Fe(OH)2(1)	-8.95	3.99	12.94	Fe(OH)2
Fe(OH)2(2)	-9.90	3.99	13.89	Fe(OH)2
FeO	-9.60	3.99	13.59	FeO
FeS(am)	-3.86	-7.64	-3.77	FeS
FeS(ppt)	-3.72	-7.64	-3.92	FeS
Fluorite	-2.28	-13.03	-10.75	CaF2
Gypsum	-3.25	-7.84	-4.59	CaSO4·2H2O
H2(g)	-7.94	-11.04	-3.10	H2
H2O(g)	-1.83	-0.00	1.83	H2O
H2S(g)	-3.66	-4.52	-0.86	H2S
Halite	-8.44	-6.89	1.55	NaCl
Hausmannite	-39.74	24.30	64.04	Mn3O4
Lepidocrocite	-8.74	7.96	16.70	FeOOH
Lime	-15.33	7.48	22.81	Ca(OH)2
Mackinawite	-3.10	-7.64	-4.53	FeS
Magnetite	-25.88	19.92	45.80	Fe3O4
Manganite	-15.92	9.42	25.34	MnOOH
Marcasite	6.75	-11.33	-18.07	FeS2
Melanterite	-8.96	-11.32	-2.36	FeSO4·7H2O
Nesquehonite	-5.97	-11.41	-5.45	MgCO3·3H2O
O2(g)	-71.33	-74.23	-2.90	O2
Pyrite	7.49	-11.33	-18.82	FeS2
Pyrochroite	-9.75	5.45	15.20	Mn(OH)2
Pyrolusite	-29.94	13.39	43.33	MnO2
Rhodochrosite	-2.38	-13.46	-11.09	MnCO3
Siderite	-4.11	-14.92	-10.82	FeCO3
Sulfur	-1.74	3.42	5.17	S
Troilite	-1.51	-7.64	-6.13	FeS

End of simulation.

Reading input data for simulation 6.

SOLUTION 1 TS-MW12 3-18-2008 (10 ft upgradient)

```

temp      13.1
pH        5.21
pe        4
redox     S(-2)/S(6)
units     mg/kgw
density   1
Cl        6.5
F         0.48
S(6)      34 as SO4
S(-2)     0.6
Ca        7.4
Fe(2)     0.005
Mg        4.9
Mn        0.12
K         1.2
Na        8.0
Alkalinity 18 as CaCO3
water     1 # kg

```

END

Beginning of initial solution calculations.

Initial solution 1. TS-MW12 3-18-2008 (10 ft upgradient)

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	3.597e-004	3.597e-004
Ca	1.846e-004	1.846e-004
Cl	1.833e-004	1.833e-004
F	2.527e-005	2.527e-005
Fe(2)	8.953e-008	8.953e-008
K	3.069e-005	3.069e-005
Mg	2.015e-004	2.015e-004
Mn	2.184e-006	2.184e-006
Na	3.480e-004	3.480e-004
S(-2)	1.871e-005	1.871e-005
S(6)	3.539e-004	3.539e-004

-----Description of solution-----

```

pH = 5.210
pe = 4.000
Activity of water = 1.000
Ionic strength = 1.900e-003
Mass of water (kg) = 1.000e+000
Total carbon (mol/kg) = 6.208e-003
Total CO2 (mol/kg) = 6.208e-003
Temperature (deg C) = 13.100
Electrical balance (eq) = -1.206e-004

```

Percent error, $100 * (Cat - |An|) / (Cat + |An|)$ = -5.07
Iterations = 8
Total H = 1.110128e+002
Total O = 5.552041e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2) / S (6)	-1.0401	-0.0591

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	6.446e-006	6.166e-006	-5.191	-5.210	-0.019
OH-	6.524e-010	6.219e-010	-9.186	-9.206	-0.021
H2O	5.551e+001	9.999e-001	1.744	-0.000	0.000
C (4)	6.208e-003				
CO2	5.842e-003	5.844e-003	-2.233	-2.233	0.000
HCO3-	3.649e-004	3.483e-004	-3.438	-3.458	-0.020
MgHCO3+	6.600e-007	6.295e-007	-6.180	-6.201	-0.021
CaHCO3+	5.398e-007	5.152e-007	-6.268	-6.288	-0.020
NaHCO3	6.488e-008	6.491e-008	-7.188	-7.188	0.000
MnHCO3+	5.571e-008	5.313e-008	-7.254	-7.275	-0.021
FeHCO3+	2.554e-009	2.436e-009	-8.593	-8.613	-0.021
CO3-2	2.413e-009	2.003e-009	-8.617	-8.698	-0.081
CaCO3	4.115e-010	4.116e-010	-9.386	-9.385	0.000
MnCO3	2.722e-010	2.724e-010	-9.565	-9.565	0.000
MgCO3	2.552e-010	2.553e-010	-9.593	-9.593	0.000
NaCO3-	6.938e-012	6.616e-012	-11.159	-11.179	-0.021
FeCO3	3.359e-012	3.361e-012	-11.474	-11.474	0.000
Fe (CO3) (OH) -	2.223e-015	2.120e-015	-14.653	-14.674	-0.021
Fe (CO3) 2-2	9.561e-018	7.909e-018	-17.019	-17.102	-0.082
Ca	1.846e-004				
Ca+2	1.768e-004	1.467e-004	-3.753	-3.834	-0.081
CaSO4	7.306e-006	7.309e-006	-5.136	-5.136	0.000
CaHCO3+	5.398e-007	5.152e-007	-6.268	-6.288	-0.020
CaF+	2.377e-008	2.266e-008	-7.624	-7.645	-0.021
CaCO3	4.115e-010	4.116e-010	-9.386	-9.385	0.000
CaHSO4+	2.430e-010	2.317e-010	-9.614	-9.635	-0.021
CaOH+	4.139e-012	3.947e-012	-11.383	-11.404	-0.021
Cl	1.833e-004				
Cl-	1.833e-004	1.748e-004	-3.737	-3.757	-0.021
MnCl+	1.278e-009	1.219e-009	-8.893	-8.914	-0.021
FeCl+	1.770e-011	1.688e-011	-10.752	-10.773	-0.021
MnCl2	9.297e-014	9.301e-014	-13.032	-13.031	0.000
MnCl3-	4.695e-018	4.478e-018	-17.328	-17.349	-0.021
F	2.527e-005				
F-	2.485e-005	2.369e-005	-4.605	-4.625	-0.021
MgF+	2.103e-007	2.005e-007	-6.677	-6.698	-0.021
HF	1.777e-007	1.778e-007	-6.750	-6.750	0.000
CaF+	2.377e-008	2.266e-008	-7.624	-7.645	-0.021

NaF	4.516e-009	4.518e-009	-8.345	-8.345	0.000
MnF+	2.942e-010	2.805e-010	-9.531	-9.552	-0.021
FeF+	1.737e-011	1.657e-011	-10.760	-10.781	-0.021
HF2-	1.517e-011	1.447e-011	-10.819	-10.840	-0.021
Fe (2)	8.953e-008				
Fe+2	8.415e-008	6.995e-008	-7.075	-7.155	-0.080
FeSO4	2.780e-009	2.781e-009	-8.556	-8.556	0.000
FeHCO3+	2.554e-009	2.436e-009	-8.593	-8.613	-0.021
FeCl+	1.770e-011	1.688e-011	-10.752	-10.773	-0.021
FeF+	1.737e-011	1.657e-011	-10.760	-10.781	-0.021
FeCO3	3.359e-012	3.361e-012	-11.474	-11.474	0.000
Fe (HS) 2	3.297e-012	3.298e-012	-11.482	-11.482	0.000
FeOH+	1.490e-012	1.421e-012	-11.827	-11.847	-0.021
FeHSO4+	1.159e-013	1.105e-013	-12.936	-12.957	-0.021
Fe (CO3) (OH) -	2.223e-015	2.120e-015	-14.653	-14.674	-0.021
Fe (HS) 3-	8.662e-017	8.260e-017	-16.062	-16.083	-0.021
Fe (CO3) 2-2	9.561e-018	7.909e-018	-17.019	-17.102	-0.082
Fe (OH) 2	4.513e-018	4.515e-018	-17.346	-17.345	0.000
H (0)	7.324e-012				
H2	3.662e-012	3.663e-012	-11.436	-11.436	0.000
K	3.069e-005				
K+	3.064e-005	2.921e-005	-4.514	-4.534	-0.021
KSO4-	4.862e-008	4.637e-008	-7.313	-7.334	-0.021
KOH	1.642e-014	1.643e-014	-13.785	-13.784	0.000
Mg	2.015e-004				
Mg+2	1.930e-004	1.604e-004	-3.714	-3.795	-0.080
MgSO4	7.658e-006	7.662e-006	-5.116	-5.116	0.000
MgHCO3+	6.600e-007	6.295e-007	-6.180	-6.201	-0.021
MgF+	2.103e-007	2.005e-007	-6.677	-6.698	-0.021
MgCO3	2.552e-010	2.553e-010	-9.593	-9.593	0.000
MgOH+	1.395e-011	1.331e-011	-10.855	-10.876	-0.021
Mn (2)	2.184e-006				
Mn+2	2.059e-006	1.712e-006	-5.686	-5.767	-0.080
MnSO4	6.736e-008	6.739e-008	-7.172	-7.171	0.000
MnHCO3+	5.571e-008	5.313e-008	-7.254	-7.275	-0.021
MnCl+	1.278e-009	1.219e-009	-8.893	-8.914	-0.021
MnF+	2.942e-010	2.805e-010	-9.531	-9.552	-0.021
MnCO3	2.722e-010	2.724e-010	-9.565	-9.565	0.000
MnOH+	2.724e-012	2.598e-012	-11.565	-11.585	-0.021
MnCl2	9.297e-014	9.301e-014	-13.032	-13.031	0.000
MnCl3-	4.695e-018	4.478e-018	-17.328	-17.349	-0.021
Mn (3)	1.209e-033				
Mn+3	1.209e-033	7.891e-034	-32.918	-33.103	-0.185
Na	3.480e-004				
Na+	3.475e-004	3.315e-004	-3.459	-3.480	-0.020
NaSO4-	4.516e-007	4.306e-007	-6.345	-6.366	-0.021
NaHCO3	6.488e-008	6.491e-008	-7.188	-7.188	0.000
NaF	4.516e-009	4.518e-009	-8.345	-8.345	0.000
NaCO3-	6.938e-012	6.616e-012	-11.159	-11.179	-0.021
NaOH	3.550e-013	3.551e-013	-12.450	-12.450	0.000
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-73.508	-73.508	0.000
S (-2)	1.871e-005				
H2S	1.847e-005	1.848e-005	-4.734	-4.733	0.000

HS-	2.413e-007	2.300e-007	-6.618	-6.638	-0.021
Fe (HS) 2	3.297e-012	3.298e-012	-11.482	-11.482	0.000
S-2	2.325e-015	1.928e-015	-14.634	-14.715	-0.081
Fe (HS) 3-	8.662e-017	8.260e-017	-16.062	-16.083	-0.021
S (6)	3.539e-004				
SO4-2	3.383e-004	2.804e-004	-3.471	-3.552	-0.081
MgSO4	7.658e-006	7.662e-006	-5.116	-5.116	0.000
CaSO4	7.306e-006	7.309e-006	-5.136	-5.136	0.000
NaSO4-	4.516e-007	4.306e-007	-6.345	-6.366	-0.021
HSO4-	1.378e-007	1.314e-007	-6.861	-6.881	-0.021
MnSO4	6.736e-008	6.739e-008	-7.172	-7.171	0.000
KSO4-	4.862e-008	4.637e-008	-7.313	-7.334	-0.021
FeSO4	2.780e-009	2.781e-009	-8.556	-8.556	0.000
CaHSO4+	2.430e-010	2.317e-010	-9.614	-9.635	-0.021
FeHSO4+	1.159e-013	1.105e-013	-12.936	-12.957	-0.021

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-12.39	10.70	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	-11.03	13.96	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-23.99	18.13	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-49.54	8.81	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-46.42	13.96	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-35.30	8.26	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-3.05	-7.39	-4.33	CaSO4
Aragonite	-4.26	-12.53	-8.27	CaCO3
Brucite	-10.17	6.63	16.79	Mg (OH) 2
Calcite	-4.11	-12.53	-8.42	CaCO3
CO2 (g)	-0.92	-2.23	-1.31	CO2
Dolomite	-8.22	-25.03	-16.80	CaMg (CO3) 2
Epsomite	-5.12	-7.35	-2.23	MgSO4:7H2O
Fe (OH) 2 (1)	-9.68	3.26	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-10.63	3.26	13.89	Fe (OH) 2
FeO	-10.33	3.26	13.59	FeO
FeS (am)	-4.81	-8.58	-3.77	FeS
FeS (ppt)	-4.67	-8.58	-3.92	FeS
Fluorite	-2.33	-13.08	-10.75	CaF2
Gypsum	-2.80	-7.39	-4.59	CaSO4:2H2O
H2 (g)	-8.34	-11.44	-3.10	H2
H2O (g)	-1.83	-0.00	1.83	H2O
H2S (g)	-3.88	-4.73	-0.86	H2S
Halite	-8.79	-7.24	1.55	NaCl
Hausmannite	-41.80	22.30	64.10	Mn3O4
Lepidocrocite	-9.27	7.43	16.70	FeOOH
Lime	-16.22	6.59	22.81	Ca (OH) 2
Mackinawite	-4.05	-8.58	-4.53	FeS
Magnetite	-27.67	18.13	45.80	Fe3O4
Manganite	-16.52	8.82	25.34	MnOOH
Marcasite	5.99	-12.09	-18.08	FeS2
Melanterite	-8.34	-10.71	-2.37	FeSO4:7H2O
Nesquehonite	-7.05	-12.49	-5.44	MgCO3:3H2O
O2 (g)	-70.60	-73.51	-2.90	O2

Pyrite	6.73	-12.09	-18.82	FeS2
Pyrochroite	-10.55	4.65	15.20	Mn (OH) 2
Pyrolusite	-30.37	12.99	43.36	MnO2
Rhodochrosite	-3.38	-14.46	-11.09	MnCO3
Siderite	-5.04	-15.85	-10.81	FeCO3
Sulfur	-1.57	3.61	5.17	S
Troilite	-2.46	-8.58	-6.13	FeS

End of simulation.

Reading input data for simulation 7.

SOLUTION 1 TS-MW06 3-18-2008 (In upgradient wall)

temp	12.5
pH	6.06
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	6.5
F	0.5
S(6)	530 as SO4
S(-2)	3.2
Ca	180
Fe(2)	2.5
Mg	27.0
Mn	0.3
K	1.8
Na	9.3
Alkalinity	356 as CaCO3
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. TS-MW06 3-18-2008 (In upgradient wall)

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	7.114e-003	7.114e-003
Ca	4.491e-003	4.491e-003
Cl	1.833e-004	1.833e-004
F	2.632e-005	2.632e-005
Fe(2)	4.477e-005	4.477e-005
K	4.603e-005	4.603e-005

Mg	1.111e-003	1.111e-003
Mn	5.461e-006	5.461e-006
Na	4.045e-004	4.045e-004
S (-2)	9.980e-005	9.980e-005
S (6)	5.517e-003	5.517e-003

-----Description of solution-----

pH	=	6.060
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	2.132e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	2.154e-002
Total CO2 (mol/kg)	=	2.154e-002
Temperature (deg C)	=	12.500
Electrical balance (eq)	=	-6.603e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	-26.20
Iterations	=	11
Total H	=	1.110197e+002
Total O	=	5.557848e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2)/S (6)	-2.0553	-0.1165

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	9.795e-007	8.710e-007	-6.009	-6.060	-0.051
OH-	4.826e-009	4.179e-009	-8.316	-8.379	-0.062
H2O	5.551e+001	9.995e-001	1.744	-0.000	0.000
C (4)	2.154e-002				
CO2	1.444e-002	1.451e-002	-1.840	-1.838	0.002
HCO3-	6.910e-003	6.046e-003	-2.161	-2.219	-0.058
CaHCO3+	1.387e-004	1.214e-004	-3.858	-3.916	-0.058
MgHCO3+	3.967e-005	3.452e-005	-4.402	-4.462	-0.060
FeHCO3+	1.113e-005	9.684e-006	-4.954	-5.014	-0.060
MnHCO3+	1.264e-006	1.099e-006	-5.898	-5.959	-0.060
NaHCO3	1.176e-006	1.181e-006	-5.930	-5.928	0.002
CaCO3	6.785e-007	6.818e-007	-6.168	-6.166	0.002
CO3-2	4.132e-007	2.422e-007	-6.384	-6.616	-0.232
MgCO3	9.626e-008	9.673e-008	-7.017	-7.014	0.002
FeCO3	9.260e-008	9.306e-008	-7.033	-7.031	0.002
MnCO3	3.906e-008	3.925e-008	-7.408	-7.406	0.002
NaCO3-	9.327e-010	8.116e-010	-9.030	-9.091	-0.060
Fe (CO3) (OH) -	4.775e-010	4.154e-010	-9.321	-9.381	-0.060
Fe (CO3) 2-2	4.620e-011	2.648e-011	-10.335	-10.577	-0.242
Ca	4.491e-003				
Ca+2	3.447e-003	2.021e-003	-2.463	-2.695	-0.232

	CaSO4	9.039e-004	9.084e-004	-3.044	-3.042	0.002
	CaHCO3+	1.387e-004	1.214e-004	-3.858	-3.916	-0.058
	CaCO3	6.785e-007	6.818e-007	-6.168	-6.166	0.002
	CaF+	3.268e-007	2.844e-007	-6.486	-6.546	-0.060
	CaHSO4+	4.649e-009	4.045e-009	-8.333	-8.393	-0.060
	CaOH+	4.423e-010	3.848e-010	-9.354	-9.415	-0.060
Cl		1.833e-004				
	Cl-	1.833e-004	1.589e-004	-3.737	-3.799	-0.062
	FeCl+	4.037e-009	3.513e-009	-8.394	-8.454	-0.060
	MnCl+	1.518e-009	1.321e-009	-8.819	-8.879	-0.060
	MnCl2	9.115e-014	9.160e-014	-13.040	-13.038	0.002
	MnCl3-	4.607e-018	4.008e-018	-17.337	-17.397	-0.060
F		2.632e-005				
	F-	2.529e-005	2.190e-005	-4.597	-4.659	-0.062
	MgF+	6.660e-007	5.795e-007	-6.177	-6.237	-0.060
	CaF+	3.268e-007	2.844e-007	-6.486	-6.546	-0.060
	HF	2.287e-008	2.298e-008	-7.641	-7.639	0.002
	NaF	4.359e-009	4.380e-009	-8.361	-8.359	0.002
	FeF+	4.032e-009	3.508e-009	-8.394	-8.455	-0.060
	MnF+	3.554e-010	3.092e-010	-9.449	-9.510	-0.060
	HF2-	1.975e-012	1.718e-012	-11.704	-11.765	-0.060
Fe (2)		4.477e-005				
	Fe+2	2.700e-005	1.602e-005	-4.569	-4.795	-0.227
	FeHCO3+	1.113e-005	9.684e-006	-4.954	-5.014	-0.060
	FeSO4	5.683e-006	5.711e-006	-5.245	-5.243	0.002
	Fe (HS) 2	8.471e-007	8.513e-007	-6.072	-6.070	0.002
	FeCO3	9.260e-008	9.306e-008	-7.033	-7.031	0.002
	FeCl+	4.037e-009	3.513e-009	-8.394	-8.454	-0.060
	FeF+	4.032e-009	3.508e-009	-8.394	-8.455	-0.060
	FeOH+	2.520e-009	2.193e-009	-8.599	-8.659	-0.060
	Fe (HS) 3-	8.227e-010	7.158e-010	-9.085	-9.145	-0.060
	Fe (CO3) (OH) -	4.775e-010	4.154e-010	-9.321	-9.381	-0.060
	Fe (CO3) 2-2	4.620e-011	2.648e-011	-10.335	-10.577	-0.242
	FeHSO4+	3.685e-011	3.206e-011	-10.434	-10.494	-0.060
	Fe (OH) 2	5.152e-014	5.177e-014	-13.288	-13.286	0.002
H (0)		1.570e-011				
	H2	7.849e-012	7.888e-012	-11.105	-11.103	0.002
K		4.603e-005				
	K+	4.539e-005	3.934e-005	-4.343	-4.405	-0.062
	KSO4-	6.439e-007	5.602e-007	-6.191	-6.252	-0.060
	KOH	1.557e-013	1.565e-013	-12.808	-12.805	0.002
Mg		1.111e-003				
	Mg+2	8.550e-004	5.071e-004	-3.068	-3.295	-0.227
	MgSO4	2.152e-004	2.162e-004	-3.667	-3.665	0.002
	MgHCO3+	3.967e-005	3.452e-005	-4.402	-4.462	-0.060
	MgF+	6.660e-007	5.795e-007	-6.177	-6.237	-0.060
	MgCO3	9.626e-008	9.673e-008	-7.017	-7.014	0.002
	MgOH+	3.226e-010	2.807e-010	-9.491	-9.552	-0.060
Mn (2)		5.461e-006				
	Mn+2	3.440e-006	2.040e-006	-5.463	-5.690	-0.227
	MnHCO3+	1.264e-006	1.099e-006	-5.898	-5.959	-0.060
	MnSO4	7.165e-007	7.200e-007	-6.145	-6.143	0.002
	MnCO3	3.906e-008	3.925e-008	-7.408	-7.406	0.002
	MnCl+	1.518e-009	1.321e-009	-8.819	-8.879	-0.060

MnF+	3.554e-010	3.092e-010	-9.449	-9.510	-0.060
MnOH+	2.388e-011	2.078e-011	-10.622	-10.682	-0.060
MnCl2	9.115e-014	9.160e-014	-13.040	-13.038	0.002
MnCl3-	4.607e-018	4.008e-018	-17.337	-17.397	-0.060
Mn (3)	2.889e-034				
Mn+3	2.889e-034	8.259e-035	-33.539	-34.083	-0.544
Na	4.045e-004				
Na+	3.987e-004	3.475e-004	-3.399	-3.459	-0.060
NaSO4-	4.690e-006	4.081e-006	-5.329	-5.389	-0.060
NaHCO3	1.176e-006	1.181e-006	-5.930	-5.928	0.002
NaF	4.359e-009	4.380e-009	-8.361	-8.359	0.002
NaCO3-	9.327e-010	8.116e-010	-9.030	-9.091	-0.060
NaOH	2.622e-012	2.635e-012	-11.581	-11.579	0.002
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-74.387	-74.385	0.002
S (-2)	9.980e-005				
H2S	8.919e-005	8.963e-005	-4.050	-4.048	0.002
HS-	8.917e-006	7.722e-006	-5.050	-5.112	-0.062
Fe (HS) 2	8.471e-007	8.513e-007	-6.072	-6.070	0.002
Fe (HS) 3-	8.227e-010	7.158e-010	-9.085	-9.145	-0.060
S-2	7.536e-013	4.382e-013	-12.123	-12.358	-0.236
S (6)	5.517e-003				
SO4-2	4.386e-003	2.545e-003	-2.358	-2.594	-0.236
CaSO4	9.039e-004	9.084e-004	-3.044	-3.042	0.002
MgSO4	2.152e-004	2.162e-004	-3.667	-3.665	0.002
FeSO4	5.683e-006	5.711e-006	-5.245	-5.243	0.002
NaSO4-	4.690e-006	4.081e-006	-5.329	-5.389	-0.060
MnSO4	7.165e-007	7.200e-007	-6.145	-6.143	0.002
KSO4-	6.439e-007	5.602e-007	-6.191	-6.252	-0.060
HSO4-	1.914e-007	1.665e-007	-6.718	-6.779	-0.060
CaHSO4+	4.649e-009	4.045e-009	-8.333	-8.393	-0.060
FeHSO4+	3.685e-011	3.206e-011	-10.434	-10.494	-0.060

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-4.44	18.65	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	0.99	25.98	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-12.14	29.98	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-25.13	33.22	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-23.14	37.24	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-20.12	23.44	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-0.95	-5.29	-4.33	CaSO4
Aragonite	-1.04	-9.31	-8.27	CaCO3
Brucite	-7.97	8.82	16.79	Mg (OH) 2
Calcite	-0.89	-9.31	-8.42	CaCO3
CO2 (g)	-0.53	-1.84	-1.31	CO2
Dolomite	-2.43	-19.22	-16.79	CaMg (CO3) 2
Epsomite	-3.66	-5.89	-2.23	MgSO4:7H2O
Fe (OH) 2 (1)	-5.62	7.32	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-6.57	7.32	13.89	Fe (OH) 2
FeO	-6.27	7.32	13.59	FeO
FeS (am)	-0.08	-3.85	-3.76	FeS

FeS (ppt)	0.07	-3.85	-3.92	FeS
Fluorite	-1.25	-12.01	-10.76	CaF2
Gypsum	-0.70	-5.29	-4.59	CaSO4:2H2O
H2 (g)	-8.01	-11.10	-3.09	H2
H2O (g)	-1.85	-0.00	1.85	H2O
H2S (g)	-3.20	-4.05	-0.85	H2S
Halite	-8.81	-7.26	1.55	NaCl
Hausmannite	-36.96	27.30	64.26	Mn3O4
Lepidocrocite	-5.37	11.33	16.70	FeOOH
Lime	-13.38	9.43	22.81	Ca (OH) 2
Mackinawite	0.68	-3.85	-4.53	FeS
Magnetite	-15.82	29.98	45.80	Fe3O4
Manganite	-14.91	10.43	25.34	MnOOH
Marcasite	11.08	-7.01	-18.09	FeS2
Melanterite	-5.02	-7.39	-2.37	FeSO4:7H2O
Nesquehonite	-4.48	-9.91	-5.44	MgCO3:3H2O
O2 (g)	-71.48	-74.38	-2.90	O2
Pyrite	11.83	-7.01	-18.84	FeS2
Pyrochroite	-8.77	6.43	15.20	Mn (OH) 2
Pyrolusite	-29.03	14.44	43.47	MnO2
Rhodochrosite	-1.22	-12.31	-11.08	MnCO3
Siderite	-0.60	-11.41	-10.81	FeCO3
Sulfur	-1.22	3.96	5.19	S
Troilite	2.28	-3.85	-6.12	FeS

End of simulation.

Reading input data for simulation 8.

SOLUTION 1 TS-MW07 3-20-2008 (Between walls)

temp	13.1
pH	5.89
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	7.9
F	0.48
S(6)	970 as SO4
S(-2)	1.3
Ca	470
Fe(2)	1.32
Mg	37.0
Mn	2.5
K	1.8
Na	12.0
Alkalinity	390 as CaCO3
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. TS-MW07 3-20-2008 (Between walls)

WARNING: Equivalent wt for alkalinity should be $\text{Ca} \cdot 5(\text{CO}_3) \cdot 5$. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	7.793e-003	7.793e-003
Ca	1.173e-002	1.173e-002
Cl	2.228e-004	2.228e-004
F	2.527e-005	2.527e-005
Fe(2)	2.364e-005	2.364e-005
K	4.603e-005	4.603e-005
Mg	1.522e-003	1.522e-003
Mn	4.551e-005	4.551e-005
Na	5.220e-004	5.220e-004
S(-2)	4.054e-005	4.054e-005
S(6)	1.010e-002	1.010e-002

-----Description of solution-----

pH	=	5.890
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	3.785e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	2.955e-002
Total CO2 (mol/kg)	=	2.955e-002
Temperature (deg C)	=	13.100
Electrical balance (eq)	=	-1.033e-003
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	-2.45
Iterations	=	11
Total H	=	1.110203e+002
Total O	=	5.561350e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-1.7919	-0.1018

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.485e-006	1.288e-006	-5.828	-5.890	-0.062
OH-	3.573e-009	2.975e-009	-8.447	-8.527	-0.080
H2O	5.551e+001	9.991e-001	1.744	-0.000	0.000
C(4)	2.955e-002				

		CO2	2.176e-002	2.195e-002	-1.662	-1.659	0.004
		HCO3-	7.391e-003	6.256e-003	-2.131	-2.204	-0.072
		CaHCO3+	3.311e-004	2.803e-004	-3.480	-3.552	-0.072
		MgHCO3+	4.935e-005	4.146e-005	-4.307	-4.382	-0.076
		MnHCO3+	9.804e-006	8.236e-006	-5.009	-5.084	-0.076
		FeHCO3+	5.568e-006	4.677e-006	-5.254	-5.330	-0.076
		NaHCO3	1.504e-006	1.517e-006	-5.823	-5.819	0.004
		CaCO3	1.062e-006	1.072e-006	-5.974	-5.970	0.004
		CO3-2	3.355e-007	1.722e-007	-6.474	-6.764	-0.290
		MnCO3	2.003e-007	2.021e-007	-6.698	-6.695	0.004
		MgCO3	7.979e-008	8.049e-008	-7.098	-7.094	0.004
		FeCO3	3.062e-008	3.089e-008	-7.514	-7.510	0.004
		NaCO3-	8.810e-010	7.400e-010	-9.055	-9.131	-0.076
		Fe (CO3) (OH) -	1.110e-010	9.320e-011	-9.955	-10.031	-0.076
		Fe (CO3) 2-2	1.255e-011	6.250e-012	-10.901	-11.204	-0.303
Ca	1.173e-002						
		Ca+2	8.639e-003	4.441e-003	-2.064	-2.352	-0.289
		CaSO4	2.755e-003	2.779e-003	-2.560	-2.556	0.004
		CaHCO3+	3.311e-004	2.803e-004	-3.480	-3.552	-0.072
		CaCO3	1.062e-006	1.072e-006	-5.974	-5.970	0.004
		CaF+	6.837e-007	5.743e-007	-6.165	-6.241	-0.076
		CaHSO4+	2.191e-008	1.841e-008	-7.659	-7.735	-0.076
		CaOH+	6.806e-010	5.717e-010	-9.167	-9.243	-0.076
Cl	2.228e-004						
		Cl-	2.228e-004	1.858e-004	-3.652	-3.731	-0.079
		MnCl+	1.331e-008	1.118e-008	-7.876	-7.952	-0.076
		FeCl+	2.282e-009	1.917e-009	-8.642	-8.717	-0.076
		MnCl2	8.985e-013	9.064e-013	-12.046	-12.043	0.004
		MnCl3-	5.521e-017	4.637e-017	-16.258	-16.334	-0.076
F	2.527e-005						
		F-	2.381e-005	1.982e-005	-4.623	-4.703	-0.080
		MgF+	7.324e-007	6.152e-007	-6.135	-6.211	-0.076
		CaF+	6.837e-007	5.743e-007	-6.165	-6.241	-0.076
		HF	3.082e-008	3.109e-008	-7.511	-7.507	0.004
		NaF	4.876e-009	4.919e-009	-8.312	-8.308	0.004
		MnF+	2.412e-009	2.026e-009	-8.618	-8.693	-0.076
		FeF+	1.764e-009	1.482e-009	-8.753	-8.829	-0.076
		HF2-	2.520e-012	2.117e-012	-11.599	-11.674	-0.076
Fe (2)	2.364e-005						
		Fe+2	1.430e-005	7.476e-006	-4.845	-5.126	-0.282
		FeHCO3+	5.568e-006	4.677e-006	-5.254	-5.330	-0.076
		FeSO4	3.699e-006	3.732e-006	-5.432	-5.428	0.004
		Fe (HS) 2	3.400e-008	3.429e-008	-7.469	-7.465	0.004
		FeCO3	3.062e-008	3.089e-008	-7.514	-7.510	0.004
		FeCl+	2.282e-009	1.917e-009	-8.642	-8.717	-0.076
		FeF+	1.764e-009	1.482e-009	-8.753	-8.829	-0.076
		FeOH+	8.646e-010	7.262e-010	-9.063	-9.139	-0.076
		Fe (CO3) (OH) -	1.110e-010	9.320e-011	-9.955	-10.031	-0.076
		FeHSO4+	3.689e-011	3.098e-011	-10.433	-10.509	-0.076
		Fe (CO3) 2-2	1.255e-011	6.250e-012	-10.901	-11.204	-0.303
		Fe (HS) 3-	1.009e-011	8.472e-012	-10.996	-11.072	-0.076
		Fe (OH) 2	1.094e-014	1.104e-014	-13.961	-13.957	0.004
H (0)	1.011e-011						
		H2	5.053e-012	5.098e-012	-11.296	-11.293	0.004

K	4.603e-005					
K+	4.514e-005	3.763e-005	-4.345	-4.424	-0.079	
KSO4-	8.929e-007	7.500e-007	-6.049	-6.125	-0.076	
KOH	1.003e-013	1.012e-013	-12.999	-12.995	0.004	
Mg	1.522e-003					
Mg+2	1.122e-003	5.880e-004	-2.950	-3.231	-0.281	
MgSO4	3.496e-004	3.527e-004	-3.456	-3.453	0.004	
MgHCO3+	4.935e-005	4.146e-005	-4.307	-4.382	-0.076	
MgF+	7.324e-007	6.152e-007	-6.135	-6.211	-0.076	
MgCO3	7.979e-008	8.049e-008	-7.098	-7.094	0.004	
MgOH+	2.777e-010	2.333e-010	-9.556	-9.632	-0.076	
Mn (2)	4.551e-005					
Mn+2	2.825e-005	1.477e-005	-4.549	-4.831	-0.282	
MnHCO3+	9.804e-006	8.236e-006	-5.009	-5.084	-0.076	
MnSO4	7.237e-006	7.301e-006	-5.140	-5.137	0.004	
MnCO3	2.003e-007	2.021e-007	-6.698	-6.695	0.004	
MnCl+	1.331e-008	1.118e-008	-7.876	-7.952	-0.076	
MnF+	2.412e-009	2.026e-009	-8.618	-8.693	-0.076	
MnOH+	1.276e-010	1.072e-010	-9.894	-9.970	-0.076	
MnCl2	8.985e-013	9.064e-013	-12.046	-12.043	0.004	
MnCl3-	5.521e-017	4.637e-017	-16.258	-16.334	-0.076	
Mn (3)	5.792e-033					
Mn+3	5.792e-033	1.206e-033	-32.237	-32.919	-0.682	
Na	5.220e-004					
Na+	5.121e-004	4.312e-004	-3.291	-3.365	-0.075	
NaSO4-	8.374e-006	7.034e-006	-5.077	-5.153	-0.076	
NaHCO3	1.504e-006	1.517e-006	-5.823	-5.819	0.004	
NaF	4.876e-009	4.919e-009	-8.312	-8.308	0.004	
NaCO3-	8.810e-010	7.400e-010	-9.055	-9.131	-0.076	
NaOH	2.190e-012	2.209e-012	-11.660	-11.656	0.004	
O (0)	0.000e+000					
O2	0.000e+000	0.000e+000	-73.799	-73.796	0.004	
S (-2)	4.054e-005					
H2S	3.775e-005	3.808e-005	-4.423	-4.419	0.004	
HS-	2.725e-006	2.269e-006	-5.565	-5.644	-0.080	
Fe (HS) 2	3.400e-008	3.429e-008	-7.469	-7.465	0.004	
Fe (HS) 3-	1.009e-011	8.472e-012	-10.996	-11.072	-0.076	
S-2	1.796e-013	9.100e-014	-12.746	-13.041	-0.295	
S (6)	1.010e-002					
SO4-2	6.972e-003	3.521e-003	-2.157	-2.453	-0.297	
CaSO4	2.755e-003	2.779e-003	-2.560	-2.556	0.004	
MgSO4	3.496e-004	3.527e-004	-3.456	-3.453	0.004	
NaSO4-	8.374e-006	7.034e-006	-5.077	-5.153	-0.076	
MnSO4	7.237e-006	7.301e-006	-5.140	-5.137	0.004	
FeSO4	3.699e-006	3.732e-006	-5.432	-5.428	0.004	
KSO4-	8.929e-007	7.500e-007	-6.049	-6.125	-0.076	
HSO4-	4.104e-007	3.447e-007	-6.387	-6.463	-0.076	
CaHSO4+	2.191e-008	1.841e-008	-7.659	-7.735	-0.076	
FeHSO4+	3.689e-011	3.098e-011	-10.433	-10.509	-0.076	

-----Saturation indices-----

Phase

SI log IAP log KT

[Fe2(OH)5]	-5.69	17.40	23.09	Fe2(OH)5
[Fe3(OH)7]	-0.93	24.06	24.99	Fe3(OH)7
[Fe3(OH)8]	-13.97	28.15	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-28.78	29.57	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-26.50	33.88	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-22.47	21.09	43.56	Fe4(OH)8(Cl)1
Anhydrite	-0.47	-4.81	-4.33	CaSO4
Aragonite	-0.85	-9.12	-8.27	CaCO3
Brucite	-8.24	8.55	16.79	Mg(OH)2
Calcite	-0.69	-9.12	-8.42	CaCO3
CO2(g)	-0.34	-1.66	-1.31	CO2
Dolomite	-2.31	-19.11	-16.80	CaMg(CO3)2
Epsomite	-3.46	-5.69	-2.23	MgSO4:7H2O
Fe(OH)2(1)	-6.29	6.65	12.94	Fe(OH)2
Fe(OH)2(2)	-7.24	6.65	13.89	Fe(OH)2
FeO	-6.94	6.65	13.59	FeO
FeS(am)	-1.11	-4.88	-3.77	FeS
FeS(ppt)	-0.97	-4.88	-3.92	FeS
Fluorite	-1.01	-11.76	-10.75	CaF2
Gypsum	-0.22	-4.81	-4.59	CaSO4:2H2O
H2(g)	-8.20	-11.29	-3.10	H2
H2O(g)	-1.83	-0.00	1.83	H2O
H2S(g)	-3.56	-4.42	-0.86	H2S
Halite	-8.65	-7.10	1.55	NaCl
Hausmannite	-35.05	29.04	64.10	Mn3O4
Lepidocrocite	-5.95	10.75	16.70	FeOOH
Lime	-13.38	9.43	22.81	Ca(OH)2
Mackinawite	-0.35	-4.88	-4.53	FeS
Magnetite	-17.64	28.16	45.80	Fe3O4
Manganite	-14.29	11.05	25.34	MnOOH
Marcasite	9.86	-8.22	-18.08	FeS2
Melanterite	-5.22	-7.58	-2.37	FeSO4:7H2O
Nesquehonite	-4.55	-10.00	-5.44	MgCO3:3H2O
O2(g)	-70.89	-73.80	-2.90	O2
Pyrite	10.60	-8.22	-18.82	FeS2
Pyrochroite	-8.25	6.95	15.20	Mn(OH)2
Pyrolusite	-28.22	15.14	43.36	MnO2
Rhodochrosite	-0.51	-11.59	-11.09	MnCO3
Siderite	-1.08	-11.89	-10.81	FeCO3
Sulfur	-1.39	3.78	5.17	S
Troilite	1.24	-4.88	-6.13	FeS

End of simulation.

Reading input data for simulation 9.

SOLUTION 1 TS-MW08 3-20-2008 (Between walls)

temp	13.5
pH	6.12
pe	4

```

redox      S(-2)/S(6)
units      mg/kgw
density    1
Cl         0.5
F          0.49
S(6)       1000 as SO4
S(-2)      51
Ca         1200
Fe(2)      0.27
Mg         83
Mn         1.8
K          43
Na         16.0
Alkalinity 640 as CaCO3
water      1 # kg

```

END

Beginning of initial solution calculations.

Initial solution 1. TS-MW08 3-20-2008 (Between walls)

WARNING: Equivalent wt for alkalinity should be $\text{Ca}_5(\text{CO}_3)_5$. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.279e-002	1.279e-002
Ca	2.994e-002	2.994e-002
Cl	1.410e-005	1.410e-005
F	2.579e-005	2.579e-005
Fe(2)	4.835e-006	4.835e-006
K	1.100e-003	1.100e-003
Mg	3.414e-003	3.414e-003
Mn	3.276e-005	3.276e-005
Na	6.960e-004	6.960e-004
S(-2)	1.591e-003	1.591e-003
S(6)	1.041e-002	1.041e-002

-----Description of solution-----

```

pH = 6.120
pe = 4.000
Activity of water = 0.999
Ionic strength = 7.278e-002
Mass of water (kg) = 1.000e+000
Total carbon (mol/kg) = 3.089e-002
Total CO2 (mol/kg) = 3.089e-002
Temperature (deg C) = 13.500
Electrical balance (eq) = 3.493e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 43.62
Iterations = 12
Total H = 1.110280e+002

```

Total O = 5.562222e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2) / S (6)	-2.3070	-0.1312

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	9.021e-007	7.586e-007	-6.045	-6.120	-0.075
OH-	6.626e-009	5.226e-009	-8.179	-8.282	-0.103
H2O	5.551e+001	9.988e-001	1.744	-0.001	0.000
C (4)	3.089e-002				
CO2	1.830e-002	1.861e-002	-1.738	-1.730	0.007
HCO3-	1.120e-002	9.076e-003	-1.951	-2.042	-0.091
CaHCO3+	1.208e-003	9.785e-004	-2.918	-3.009	-0.091
MgHCO3+	1.578e-004	1.267e-004	-3.802	-3.897	-0.095
MnHCO3+	9.118e-006	7.321e-006	-5.040	-5.135	-0.095
CaCO3	6.280e-006	6.386e-006	-5.202	-5.195	0.007
NaHCO3	2.770e-006	2.817e-006	-5.558	-5.550	0.007
CO3-2	9.955e-007	4.289e-007	-6.002	-6.368	-0.366
MgCO3	4.176e-007	4.247e-007	-6.379	-6.372	0.007
MnCO3	3.032e-007	3.083e-007	-6.518	-6.511	0.007
FeHCO3+	2.401e-007	1.928e-007	-6.620	-6.715	-0.095
NaCO3-	3.003e-009	2.411e-009	-8.522	-8.618	-0.095
FeCO3	2.149e-009	2.186e-009	-8.668	-8.660	0.007
Fe (CO3) (OH) -	1.394e-011	1.120e-011	-10.856	-10.951	-0.095
Fe (CO3) 2-2	2.650e-012	1.101e-012	-11.577	-11.958	-0.381
Ca	2.994e-002				
Ca+2	2.439e-002	1.058e-002	-1.613	-1.975	-0.363
CaSO4	4.332e-003	4.405e-003	-2.363	-2.356	0.007
CaHCO3+	1.208e-003	9.785e-004	-2.918	-3.009	-0.091
CaCO3	6.280e-006	6.386e-006	-5.202	-5.195	0.007
CaF+	1.558e-006	1.251e-006	-5.808	-5.903	-0.095
CaHSO4+	2.148e-008	1.724e-008	-7.668	-7.763	-0.095
CaOH+	2.880e-009	2.313e-009	-8.541	-8.636	-0.095
Cl	1.410e-005				
Cl-	1.410e-005	1.115e-005	-4.851	-4.953	-0.102
MnCl+	5.120e-010	4.111e-010	-9.291	-9.386	-0.095
FeCl+	4.072e-012	3.270e-012	-11.390	-11.485	-0.095
MnCl2	1.968e-015	2.001e-015	-14.706	-14.699	0.007
MnCl3-	7.653e-021	6.145e-021	-20.116	-20.211	-0.095
F	2.579e-005				
F-	2.274e-005	1.793e-005	-4.643	-4.746	-0.103
CaF+	1.558e-006	1.251e-006	-5.808	-5.903	-0.095
MgF+	1.471e-006	1.181e-006	-5.832	-5.928	-0.095
HF	1.639e-008	1.667e-008	-7.785	-7.778	0.007
NaF	5.601e-009	5.695e-009	-8.252	-8.244	0.007
MnF+	1.398e-009	1.123e-009	-8.854	-8.950	-0.095
FeF+	4.745e-011	3.810e-011	-10.324	-10.419	-0.095

HF2-	1.285e-012	1.032e-012	-11.891	-11.986	-0.095
Fe (2)	4.835e-006				
Fe (HS) 2	3.964e-006	4.031e-006	-5.402	-5.395	0.007
Fe+2	4.789e-007	2.124e-007	-6.320	-6.673	-0.353
FeHCO3+	2.401e-007	1.928e-007	-6.620	-6.715	-0.095
Fe (HS) 3-	7.977e-008	6.405e-008	-7.098	-7.194	-0.095
FeSO4	6.963e-008	7.081e-008	-7.157	-7.150	0.007
FeCO3	2.149e-009	2.186e-009	-8.668	-8.660	0.007
FeF+	4.745e-011	3.810e-011	-10.324	-10.419	-0.095
FeOH+	4.507e-011	3.619e-011	-10.346	-10.441	-0.095
Fe (CO3) (OH) -	1.394e-011	1.120e-011	-10.856	-10.951	-0.095
FeCl+	4.072e-012	3.270e-012	-11.390	-11.485	-0.095
Fe (CO3) 2-2	2.650e-012	1.101e-012	-11.577	-11.958	-0.381
FeHSO4+	4.311e-013	3.461e-013	-12.365	-12.461	-0.095
Fe (OH) 2	8.890e-016	9.040e-016	-15.051	-15.044	0.007
H (0)	3.710e-011				
H2	1.855e-011	1.886e-011	-10.732	-10.724	0.007
K	1.100e-003				
K+	1.085e-003	8.582e-004	-2.964	-3.066	-0.102
KSO4-	1.422e-005	1.142e-005	-4.847	-4.942	-0.095
KOH	3.853e-012	3.918e-012	-11.414	-11.407	0.007
Mg	3.414e-003				
Mg+2	2.765e-003	1.238e-003	-2.558	-2.907	-0.349
MgSO4	4.892e-004	4.975e-004	-3.310	-3.303	0.007
MgHCO3+	1.578e-004	1.267e-004	-3.802	-3.897	-0.095
MgF+	1.471e-006	1.181e-006	-5.832	-5.928	-0.095
MgCO3	4.176e-007	4.247e-007	-6.379	-6.372	0.007
MgOH+	1.080e-009	8.672e-010	-8.967	-9.062	-0.095
Mn (2)	3.276e-005				
Mn+2	2.040e-005	9.050e-006	-4.690	-5.043	-0.353
MnHCO3+	9.118e-006	7.321e-006	-5.040	-5.135	-0.095
MnSO4	2.938e-006	2.988e-006	-5.532	-5.525	0.007
MnCO3	3.032e-007	3.083e-007	-6.518	-6.511	0.007
MnF+	1.398e-009	1.123e-009	-8.854	-8.950	-0.095
MnCl+	5.120e-010	4.111e-010	-9.291	-9.386	-0.095
MnOH+	1.439e-010	1.155e-010	-9.842	-9.937	-0.095
MnCl2	1.968e-015	2.001e-015	-14.706	-14.699	0.007
MnCl3-	7.653e-021	6.145e-021	-20.116	-20.211	-0.095
Mn (3)	1.734e-033				
Mn+3	1.734e-033	2.405e-034	-32.761	-33.619	-0.858
Na	6.960e-004				
Na+	6.857e-004	5.519e-004	-3.164	-3.258	-0.094
NaSO4-	7.449e-006	5.981e-006	-5.128	-5.223	-0.095
NaHCO3	2.770e-006	2.817e-006	-5.558	-5.550	0.007
NaF	5.601e-009	5.695e-009	-8.252	-8.244	0.007
NaCO3-	3.003e-009	2.411e-009	-8.522	-8.618	-0.095
NaOH	4.721e-012	4.801e-012	-11.326	-11.319	0.007
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-74.800	-74.793	0.007
S (-2)	1.591e-003				
H2S	1.397e-003	1.421e-003	-2.855	-2.847	0.007
HS-	1.850e-004	1.459e-004	-3.733	-3.836	-0.103
Fe (HS) 2	3.964e-006	4.031e-006	-5.402	-5.395	0.007
Fe (HS) 3-	7.977e-008	6.405e-008	-7.098	-7.194	-0.095

S-2	2.426e-011	1.024e-011	-10.615	-10.990	-0.375
S (6)	1.041e-002				
SO4-2	5.564e-003	2.333e-003	-2.255	-2.632	-0.378
CaSO4	4.332e-003	4.405e-003	-2.363	-2.356	0.007
MgSO4	4.892e-004	4.975e-004	-3.310	-3.303	0.007
KSO4-	1.422e-005	1.142e-005	-4.847	-4.942	-0.095
NaSO4-	7.449e-006	5.981e-006	-5.128	-5.223	-0.095
MnSO4	2.938e-006	2.988e-006	-5.532	-5.525	0.007
HSO4-	1.688e-007	1.355e-007	-6.773	-6.868	-0.095
FeSO4	6.963e-008	7.081e-008	-7.157	-7.150	0.007
CaHSO4+	2.148e-008	1.724e-008	-7.668	-7.763	-0.095
FeHSO4+	4.311e-013	3.461e-013	-12.365	-12.461	-0.095

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH) 5]	-8.15	14.94	23.09	Fe2(OH) 5
[Fe3(OH) 7]	-4.48	20.51	24.99	Fe3(OH) 7
[Fe3(OH) 8]	-17.80	24.32	42.12	Fe3(OH) 8
[Fe6(OH) 12] [CO3]	-35.93	22.42	58.35	Fe6(OH) 12 (CO3) 1
[Fe6(OH) 12] [SO4]	-34.23	26.15	60.38	Fe6(OH) 12 (SO4) 1
[Fe6(OH) 8] [Cl]	-28.56	15.00	43.56	Fe4(OH) 8 (Cl) 1
Anhydrite	-0.27	-4.61	-4.33	CaSO4
Aragonite	-0.07	-8.34	-8.27	CaCO3
Brucite	-7.46	9.33	16.79	Mg(OH) 2
Calcite	0.08	-8.34	-8.42	CaCO3
CO2 (g)	-0.41	-1.73	-1.32	CO2
Dolomite	-0.81	-17.62	-16.81	CaMg (CO3) 2
Epsomite	-3.32	-5.54	-2.22	MgSO4:7H2O
Fe(OH) 2 (1)	-7.37	5.57	12.94	Fe(OH) 2
Fe(OH) 2 (2)	-8.32	5.57	13.89	Fe(OH) 2
FeO	-8.02	5.57	13.59	FeO
FeS (am)	-0.61	-4.39	-3.78	FeS
FeS (ppt)	-0.47	-4.39	-3.92	FeS
Fluorite	-0.72	-11.47	-10.75	CaF2
Gypsum	-0.02	-4.61	-4.59	CaSO4:2H2O
H2 (g)	-7.63	-10.72	-3.10	H2
H2O (g)	-1.82	-0.00	1.82	H2O
H2S (g)	-1.98	-2.85	-0.86	H2S
Halite	-9.77	-8.21	1.56	NaCl
Hausmannite	-34.78	29.21	63.99	Mn3O4
Lepidocrocite	-7.32	9.38	16.70	FeOOH
Lime	-12.55	10.26	22.81	Ca (OH) 2
Mackinawite	0.15	-4.39	-4.54	FeS
Magnetite	-21.47	24.33	45.80	Fe3O4
Manganite	-14.33	11.01	25.34	MnOOH
Marcasite	11.35	-6.72	-18.07	FeS2
Melanterite	-6.95	-9.31	-2.36	FeSO4:7H2O
Nesquehonite	-3.83	-9.28	-5.45	MgCO3:3H2O
O2 (g)	-71.89	-74.79	-2.91	O2
Pyrite	12.09	-6.72	-18.81	FeS2
Pyrochroite	-8.00	7.20	15.20	Mn (OH) 2
Pyrolusite	-28.47	14.82	43.29	MnO2

Rhodochrosite	-0.32	-11.41	-11.09	MnCO3
Siderite	-2.22	-13.04	-10.82	FeCO3
Sulfur	-0.38	4.78	5.16	S
Troilite	1.74	-4.39	-6.13	FeS

End of simulation.

Reading input data for simulation 10.

SOLUTION 1 TS-MW09 3-17-2008 (15 ft downgradient)

temp	13.6
pH	5.50
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	7.1
F	0.56
S(6)	430 as SO4
S(-2)	0.6
Ca	93
Fe(2)	1.82
Mg	53
Mn	1.2
K	1.6
Na	13.0
Alkalinity	2.8 as CaCO3
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. TS-MW09 3-17-2008 (15 ft downgradient)

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	5.595e-005	5.595e-005
Ca	2.320e-003	2.320e-003
Cl	2.003e-004	2.003e-004
F	2.948e-005	2.948e-005
Fe(2)	3.259e-005	3.259e-005
K	4.092e-005	4.092e-005
Mg	2.180e-003	2.180e-003
Mn	2.184e-005	2.184e-005
Na	5.655e-004	5.655e-004

S(-2)	1.871e-005	1.871e-005
S(6)	4.476e-003	4.476e-003

-----Description of solution-----

pH	=	5.500
pe	=	4.000
Activity of water	=	1.000
Ionic strength	=	1.489e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	4.988e-004
Total CO2 (mol/kg)	=	4.988e-004
Temperature (deg C)	=	13.600
Electrical balance (eq)	=	4.779e-004
Percent error, 100*(Cat- An)/(Cat+ An)	=	3.11
Iterations	=	8
Total H	=	1.110125e+002
Total O	=	5.552518e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-1.3004	-0.0740

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.507e-006	3.162e-006	-5.455	-5.500	-0.045
OH-	1.432e-009	1.266e-009	-8.844	-8.898	-0.054
H2O	5.551e+001	9.998e-001	1.744	-0.000	0.000
C(4)	4.988e-004				
CO2	4.391e-004	4.406e-004	-3.357	-3.356	0.001
HCO3-	5.805e-005	5.171e-005	-4.236	-4.286	-0.050
MgHCO3+	7.311e-007	6.484e-007	-6.136	-6.188	-0.052
CaHCO3+	6.922e-007	6.166e-007	-6.160	-6.210	-0.050
FeHCO3+	1.001e-007	8.874e-008	-7.000	-7.052	-0.052
MnHCO3+	5.988e-008	5.310e-008	-7.223	-7.275	-0.052
NaHCO3	1.440e-008	1.445e-008	-7.842	-7.840	0.001
CaCO3	9.632e-010	9.665e-010	-9.016	-9.015	0.001
CO3-2	9.334e-010	5.877e-010	-9.030	-9.231	-0.201
MnCO3	5.361e-010	5.379e-010	-9.271	-9.269	0.001
MgCO3	5.215e-010	5.233e-010	-9.283	-9.281	0.001
FeCO3	2.411e-010	2.419e-010	-9.618	-9.616	0.001
NaCO3-	3.373e-012	2.992e-012	-11.472	-11.524	-0.052
Fe(CO3)(OH)-	3.356e-013	2.976e-013	-12.474	-12.526	-0.052
Fe(CO3)2-2	2.701e-016	1.671e-016	-15.568	-15.777	-0.209
Ca	2.320e-003				
Ca+2	1.856e-003	1.168e-003	-2.731	-2.933	-0.201
CaSO4	4.637e-004	4.653e-004	-3.334	-3.332	0.001
CaHCO3+	6.922e-007	6.166e-007	-6.160	-6.210	-0.050
CaF+	2.117e-007	1.878e-007	-6.674	-6.726	-0.052

	CaHSO4+	8.571e-009	7.601e-009	-8.067	-8.119	-0.052
	CaCO3	9.632e-010	9.665e-010	-9.016	-9.015	0.001
	CaOH+	6.910e-011	6.128e-011	-10.161	-10.213	-0.052
Cl	2.003e-004					
	Cl-	2.003e-004	1.771e-004	-3.698	-3.752	-0.053
	MnCl+	9.375e-009	8.314e-009	-8.028	-8.080	-0.052
	FeCl+	4.731e-009	4.196e-009	-8.325	-8.377	-0.052
	MnCl2	6.405e-013	6.427e-013	-12.193	-12.192	0.001
	MnCl3-	3.535e-017	3.135e-017	-16.452	-16.504	-0.052
F	2.948e-005					
	F-	2.753e-005	2.434e-005	-4.560	-4.614	-0.054
	MgF+	1.626e-006	1.442e-006	-5.789	-5.841	-0.052
	CaF+	2.117e-007	1.878e-007	-6.674	-6.726	-0.052
	HF	9.415e-008	9.447e-008	-7.026	-7.025	0.001
	NaF	6.937e-009	6.960e-009	-8.159	-8.157	0.001
	FeF+	4.709e-009	4.176e-009	-8.327	-8.379	-0.052
	MnF+	2.188e-009	1.940e-009	-8.660	-8.712	-0.052
	HF2-	8.955e-012	7.942e-012	-11.048	-11.100	-0.052
Fe (2)	3.259e-005					
	Fe+2	2.701e-005	1.716e-005	-4.568	-4.765	-0.197
	FeSO4	5.462e-006	5.481e-006	-5.263	-5.261	0.001
	FeHCO3+	1.001e-007	8.874e-008	-7.000	-7.052	-0.052
	FeCl+	4.731e-009	4.196e-009	-8.325	-8.377	-0.052
	FeF+	4.709e-009	4.176e-009	-8.327	-8.379	-0.052
	Fe (HS) 2	3.106e-009	3.116e-009	-8.508	-8.506	0.001
	FeOH+	7.980e-010	7.077e-010	-9.098	-9.150	-0.052
	FeCO3	2.411e-010	2.419e-010	-9.618	-9.616	0.001
	FeHSO4+	1.259e-010	1.117e-010	-9.900	-9.952	-0.052
	Fe (CO3) (OH) -	3.356e-013	2.976e-013	-12.474	-12.526	-0.052
	Fe (HS) 3-	1.727e-013	1.532e-013	-12.763	-12.815	-0.052
	Fe (OH) 2	4.197e-015	4.211e-015	-14.377	-14.376	0.001
	Fe (CO3) 2-2	2.701e-016	1.671e-016	-15.568	-15.777	-0.209
H (0)	6.333e-012					
	H2	3.167e-012	3.178e-012	-11.499	-11.498	0.001
K	4.092e-005					
	K+	4.041e-005	3.574e-005	-4.394	-4.447	-0.053
	KSO4-	5.136e-007	4.555e-007	-6.289	-6.342	-0.052
	KOH	3.904e-014	3.918e-014	-13.408	-13.407	0.001
Mg	2.180e-003					
	Mg+2	1.751e-003	1.112e-003	-2.757	-2.954	-0.197
	MgSO4	4.269e-004	4.284e-004	-3.370	-3.368	0.001
	MgF+	1.626e-006	1.442e-006	-5.789	-5.841	-0.052
	MgHCO3+	7.311e-007	6.484e-007	-6.136	-6.188	-0.052
	MgCO3	5.215e-010	5.233e-010	-9.283	-9.281	0.001
	MgOH+	2.129e-010	1.888e-010	-9.672	-9.724	-0.052
Mn (2)	2.184e-005					
	Mn+2	1.814e-005	1.152e-005	-4.741	-4.938	-0.197
	MnSO4	3.633e-006	3.646e-006	-5.440	-5.438	0.001
	MnHCO3+	5.988e-008	5.310e-008	-7.223	-7.275	-0.052
	MnCl+	9.375e-009	8.314e-009	-8.028	-8.080	-0.052
	MnF+	2.188e-009	1.940e-009	-8.660	-8.712	-0.052
	MnCO3	5.361e-010	5.379e-010	-9.271	-9.269	0.001
	MnOH+	4.018e-011	3.563e-011	-10.396	-10.448	-0.052
	MnCl2	6.405e-013	6.427e-013	-12.193	-12.192	0.001

MnCl3-	3.535e-017	3.135e-017	-16.452	-16.504	-0.052
Mn (3)	9.306e-033				
Mn+3	9.306e-033	3.157e-033	-32.031	-32.501	-0.469
Na	5.655e-004				
Na+	5.596e-004	4.970e-004	-3.252	-3.304	-0.052
NaSO4-	5.812e-006	5.155e-006	-5.236	-5.288	-0.052
NaHCO3	1.440e-008	1.445e-008	-7.842	-7.840	0.001
NaF	6.937e-009	6.960e-009	-8.159	-8.157	0.001
NaCO3-	3.373e-012	2.992e-012	-11.472	-11.524	-0.052
NaOH	1.035e-012	1.038e-012	-11.985	-11.984	0.001
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-73.211	-73.210	0.001
S (-2)	1.871e-005				
H2S	1.820e-005	1.826e-005	-4.740	-4.739	0.001
HS-	5.106e-007	4.514e-007	-6.292	-6.345	-0.054
Fe (HS) 2	3.106e-009	3.116e-009	-8.508	-8.506	0.001
Fe (HS) 3-	1.727e-013	1.532e-013	-12.763	-12.815	-0.052
S-2	1.223e-014	7.655e-015	-13.912	-14.116	-0.204
S (6)	4.476e-003				
SO4-2	3.570e-003	2.231e-003	-2.447	-2.652	-0.204
CaSO4	4.637e-004	4.653e-004	-3.334	-3.332	0.001
MgSO4	4.269e-004	4.284e-004	-3.370	-3.368	0.001
NaSO4-	5.812e-006	5.155e-006	-5.236	-5.288	-0.052
FeSO4	5.462e-006	5.481e-006	-5.263	-5.261	0.001
MnSO4	3.633e-006	3.646e-006	-5.440	-5.438	0.001
HSO4-	6.104e-007	5.413e-007	-6.214	-6.267	-0.052
KSO4-	5.136e-007	4.555e-007	-6.289	-6.342	-0.052
CaHSO4+	8.571e-009	7.601e-009	-8.067	-8.119	-0.052
FeHSO4+	1.259e-010	1.117e-010	-9.900	-9.952	-0.052

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH)5]	-6.42	16.67	23.09	Fe2(OH)5
[Fe3(OH)7]	-2.09	22.90	24.99	Fe3(OH)7
[Fe3(OH)8]	-15.02	27.10	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-32.78	25.57	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-28.23	32.15	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-23.67	19.89	43.56	Fe4(OH)8(Cl)1
Anhydrite	-1.25	-5.58	-4.33	CaSO4
Aragonite	-3.89	-12.16	-8.27	CaCO3
Brucite	-8.75	8.05	16.79	Mg(OH)2
Calcite	-3.74	-12.16	-8.42	CaCO3
CO2(g)	-2.03	-3.36	-1.32	CO2
Dolomite	-7.53	-24.35	-16.82	CaMg(CO3)2
Epsomite	-3.38	-5.61	-2.22	MgSO4:7H2O
Fe(OH)2(1)	-6.71	6.23	12.94	Fe(OH)2
Fe(OH)2(2)	-7.66	6.23	13.89	Fe(OH)2
FeO	-7.36	6.23	13.59	FeO
FeS(am)	-1.83	-5.61	-3.78	FeS
FeS(ppt)	-1.70	-5.61	-3.92	FeS
Fluorite	-1.42	-12.16	-10.74	CaF2
Gypsum	-1.00	-5.58	-4.59	CaSO4:2H2O

H2 (g)	-8.40	-11.50	-3.10	H2
H2O (g)	-1.82	-0.00	1.82	H2O
H2S (g)	-3.87	-4.74	-0.86	H2S
Halite	-8.61	-7.06	1.56	NaCl
Hausmannite	-37.38	26.58	63.96	Mn3O4
Lepidocrocite	-6.27	10.43	16.70	FeOOH
Lime	-14.74	8.07	22.81	Ca (OH) 2
Mackinawite	-1.07	-5.61	-4.54	FeS
Magnetite	-18.70	27.10	45.80	Fe3O4
Manganite	-15.08	10.26	25.34	MnOOH
Marcasite	9.01	-9.06	-18.06	FeS2
Melanterite	-5.06	-7.42	-2.36	FeSO4:7H2O
Nesquehonite	-6.73	-12.19	-5.45	MgCO3:3H2O
O2 (g)	-70.30	-73.21	-2.91	O2
Pyrite	9.75	-9.06	-18.81	FeS2
Pyrochroite	-9.14	6.06	15.20	Mn (OH) 2
Pyrolusite	-28.82	14.46	43.28	MnO2
Rhodochrosite	-3.08	-14.17	-11.09	MnCO3
Siderite	-3.18	-14.00	-10.82	FeCO3
Sulfur	-1.50	3.66	5.16	S
Troilite	0.52	-5.61	-6.13	FeS

End of simulation.

Reading input data for simulation 11.

End of run.

Seneca Depot

Input file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\Seneca.pqi
Output file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\Seneca.pgo
Database file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\phreeqc8.dat

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\phreeqc8.dat

SOLUTION 1 MWT-25 1-10-08 (upgradient of Biowall A)

temp	25
pH	7.15
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	33
F	0.6
S(6)	190 as SO4
S(-2)	1.3 as S
N(5)	1.2
N(3)	0.25
Ca	160
Fe	0.057
Mg	33
Mn	0.36
K	13
Na	48
Alkalinity	850 as HCO3
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. MWT-25 1-10-08 (upgradient of Biowall A)

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.393e-002	1.393e-002
Ca	3.992e-003	3.992e-003
Cl	9.308e-004	9.308e-004
F	3.158e-005	3.158e-005
Fe	1.021e-006	1.021e-006
K	3.325e-004	3.325e-004
Mg	1.357e-003	1.357e-003
Mn	6.553e-006	6.553e-006
N(3)	1.785e-005	1.785e-005
N(5)	8.567e-005	8.567e-005
Na	2.088e-003	2.088e-003
S(-2)	4.054e-005	4.054e-005
S(6)	1.978e-003	1.978e-003

-----Description of solution-----

pH	=	7.150
pe	=	4.000
Activity of water	=	1.000
Ionic strength	=	2.052e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	1.571e-002
Total CO2 (mol/kg)	=	1.571e-002
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	-5.817e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	-19.94
Iterations	=	9
Total H	=	1.110263e+002
Total O	=	5.555970e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
N(3)/N(5)	7.4757	0.4422
S(-2)/S(6)	-3.6393	-0.2153

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	1.633e-007	1.413e-007	-6.787	-6.850	-0.063
H+	7.966e-008	7.079e-008	-7.099	-7.150	-0.051
H2O	5.551e+001	9.996e-001	1.744	-0.000	0.000
C(4)	1.571e-002				
HCO3-	1.337e-002	1.169e-002	-1.874	-1.932	-0.058
CO2	1.853e-003	1.862e-003	-2.732	-2.730	0.002
CaHCO3+	3.296e-004	2.882e-004	-3.482	-3.540	-0.058
MgHCO3+	1.037e-004	9.019e-005	-3.984	-4.045	-0.061

	CaCO3	2.502e-005	2.514e-005	-4.602	-4.600	0.002
	CO3-2	1.323e-005	7.744e-006	-4.878	-5.111	-0.233
	NaHCO3	1.178e-005	1.184e-005	-4.929	-4.927	0.002
	MgCO3	4.849e-006	4.872e-006	-5.314	-5.312	0.002
	MnHCO3+	2.147e-006	1.867e-006	-5.668	-5.729	-0.061
	MnCO3	1.097e-006	1.102e-006	-5.960	-5.958	0.002
	NaCO3-	2.986e-007	2.597e-007	-6.525	-6.586	-0.061
	FeHCO3+	2.344e-007	2.039e-007	-6.630	-6.691	-0.061
	FeCO3	3.224e-008	3.240e-008	-7.492	-7.490	0.002
	Fe (CO3) (OH) -	2.046e-009	1.780e-009	-8.689	-8.750	-0.061
	Fe (CO3) 2-2	5.155e-010	2.948e-010	-9.288	-9.531	-0.243
Ca		3.992e-003				
	Ca+2	3.304e-003	1.932e-003	-2.481	-2.714	-0.233
	CaSO4	3.334e-004	3.349e-004	-3.477	-3.475	0.002
	CaHCO3+	3.296e-004	2.882e-004	-3.482	-3.540	-0.058
	CaCO3	2.502e-005	2.514e-005	-4.602	-4.600	0.002
	CaF+	4.987e-007	4.336e-007	-6.302	-6.363	-0.061
	CaOH+	5.207e-009	4.528e-009	-8.283	-8.344	-0.061
	CaHSO4+	1.597e-010	1.389e-010	-9.797	-9.857	-0.061
Cl		9.308e-004				
	Cl-	9.308e-004	8.063e-004	-3.031	-3.093	-0.062
	MnCl+	6.768e-009	5.885e-009	-8.170	-8.230	-0.061
	FeCl+	2.232e-010	1.941e-010	-9.651	-9.712	-0.061
	MnCl2	2.062e-012	2.072e-012	-11.686	-11.684	0.002
	MnCl3-	5.291e-016	4.601e-016	-15.277	-15.337	-0.061
	FeCl+2	1.627e-025	9.305e-026	-24.789	-25.031	-0.243
	FeCl2+	3.854e-028	3.351e-028	-27.414	-27.475	-0.061
	FeCl3	2.690e-032	2.702e-032	-31.570	-31.568	0.002
F		3.158e-005				
	F-	2.976e-005	2.576e-005	-4.526	-4.589	-0.063
	MgF+	1.291e-006	1.122e-006	-5.889	-5.950	-0.061
	CaF+	4.987e-007	4.336e-007	-6.302	-6.363	-0.061
	NaF	2.657e-008	2.670e-008	-7.576	-7.574	0.002
	HF	2.723e-009	2.736e-009	-8.565	-8.563	0.002
	MnF+	3.672e-010	3.194e-010	-9.435	-9.496	-0.061
	FeF+	5.167e-011	4.493e-011	-10.287	-10.347	-0.061
	HF2-	3.110e-013	2.704e-013	-12.507	-12.568	-0.061
	FeF+2	2.729e-022	1.560e-022	-21.564	-21.807	-0.243
	FeF2+	1.840e-022	1.600e-022	-21.735	-21.796	-0.061
	FeF3	6.505e-024	6.535e-024	-23.187	-23.185	0.002
Fe (2)		1.021e-006				
	FeS	3.496e-007	3.513e-007	-6.456	-6.454	0.002
	Fe+2	2.945e-007	1.744e-007	-6.531	-6.758	-0.228
	FeHCO3+	2.344e-007	2.039e-007	-6.630	-6.691	-0.061
	Fe (HS) 2	7.903e-008	7.941e-008	-7.102	-7.100	0.002
	FeCO3	3.224e-008	3.240e-008	-7.492	-7.490	0.002
	FeSO4	2.681e-008	2.694e-008	-7.572	-7.570	0.002
	Fe (CO3) (OH) -	2.046e-009	1.780e-009	-8.689	-8.750	-0.061
	FeOH+	8.954e-010	7.786e-010	-9.048	-9.109	-0.061
	Fe (CO3) 2-2	5.155e-010	2.948e-010	-9.288	-9.531	-0.243
	Fe (HS) 3-	2.248e-010	1.954e-010	-9.648	-9.709	-0.061
	FeCl+	2.232e-010	1.941e-010	-9.651	-9.712	-0.061
	FeF+	5.167e-011	4.493e-011	-10.287	-10.347	-0.061
	Fe (OH) 2	8.493e-014	8.534e-014	-13.071	-13.069	0.002

FeHSO4+	1.442e-014	1.254e-014	-13.841	-13.902	-0.061
Fe (3)	4.866e-015				
Fe (OH) 3	2.948e-015	2.962e-015	-14.530	-14.528	0.002
Fe (OH) 2+	1.873e-015	1.629e-015	-14.728	-14.788	-0.061
Fe (OH) 4-	4.386e-017	3.814e-017	-16.358	-16.419	-0.061
FeOH+2	6.091e-019	3.483e-019	-18.215	-18.458	-0.243
FeF+2	2.729e-022	1.560e-022	-21.564	-21.807	-0.243
FeF2+	1.840e-022	1.600e-022	-21.735	-21.796	-0.061
FeSO4+	4.185e-023	3.640e-023	-22.378	-22.439	-0.061
Fe+3	1.105e-023	3.821e-024	-22.956	-23.418	-0.461
FeF3	6.505e-024	6.535e-024	-23.187	-23.185	0.002
Fe (SO4) 2-	7.954e-025	6.917e-025	-24.099	-24.160	-0.061
FeCl+2	1.627e-025	9.305e-026	-24.789	-25.031	-0.243
FeCl2+	3.854e-028	3.351e-028	-27.414	-27.475	-0.061
FeHSO4+2	1.207e-029	6.900e-030	-28.918	-29.161	-0.243
FeCl3	2.690e-032	2.702e-032	-31.570	-31.568	0.002
Fe2 (OH) 2+4	3.054e-035	3.266e-036	-34.515	-35.486	-0.971
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-46.437	-47.954	-1.517
H (0)	1.342e-010				
H2	6.708e-011	6.740e-011	-10.173	-10.171	0.002
K	3.325e-004				
K+	3.305e-004	2.863e-004	-3.481	-3.543	-0.062
KSO4-	2.009e-006	1.747e-006	-5.697	-5.758	-0.061
KOH	1.395e-011	1.401e-011	-10.855	-10.853	0.002
Mg	1.357e-003				
Mg+2	1.114e-003	6.593e-004	-2.953	-3.181	-0.228
MgSO4	1.336e-004	1.343e-004	-3.874	-3.872	0.002
MgHCO3+	1.037e-004	9.019e-005	-3.984	-4.045	-0.061
MgCO3	4.849e-006	4.872e-006	-5.314	-5.312	0.002
MgF+	1.291e-006	1.122e-006	-5.889	-5.950	-0.061
MgOH+	1.677e-008	1.458e-008	-7.775	-7.836	-0.061
Mn (2)	6.553e-006				
Mn+2	3.026e-006	1.792e-006	-5.519	-5.747	-0.228
MnHCO3+	2.147e-006	1.867e-006	-5.668	-5.729	-0.061
MnCO3	1.097e-006	1.102e-006	-5.960	-5.958	0.002
MnSO4	2.755e-007	2.768e-007	-6.560	-6.558	0.002
MnCl+	6.768e-009	5.885e-009	-8.170	-8.230	-0.061
MnOH+	7.477e-010	6.502e-010	-9.126	-9.187	-0.061
MnF+	3.672e-010	3.194e-010	-9.435	-9.496	-0.061
MnCl2	2.062e-012	2.072e-012	-11.686	-11.684	0.002
Mn (NO3) 2	3.882e-014	3.900e-014	-13.411	-13.409	0.002
MnCl3-	5.291e-016	4.601e-016	-15.277	-15.337	-0.061
Mn (3)	4.467e-035				
Mn+3	4.467e-035	1.270e-035	-34.350	-34.896	-0.546
N (3)	1.785e-005				
NO2-	1.785e-005	1.541e-005	-4.748	-4.812	-0.064
N (5)	8.567e-005				
NO3-	8.567e-005	7.395e-005	-4.067	-4.131	-0.064
Mn (NO3) 2	3.882e-014	3.900e-014	-13.411	-13.409	0.002
Na	2.088e-003				
Na+	2.067e-003	1.801e-003	-2.685	-2.745	-0.060
NaHCO3	1.178e-005	1.184e-005	-4.929	-4.927	0.002
NaSO4-	9.015e-006	7.840e-006	-5.045	-5.106	-0.061
NaCO3-	2.986e-007	2.597e-007	-6.525	-6.586	-0.061

NaF	2.657e-008	2.670e-008	-7.576	-7.574	0.002
NaOH	1.672e-010	1.680e-010	-9.777	-9.775	0.002
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-72.040	-72.038	0.002
S (-2)	4.054e-005				
HS-	2.611e-005	2.260e-005	-4.583	-4.646	-0.063
H2S	1.393e-005	1.399e-005	-4.856	-4.854	0.002
FeS	3.496e-007	3.513e-007	-6.456	-6.454	0.002
Fe (HS) 2	7.903e-008	7.941e-008	-7.102	-7.100	0.002
Fe (HS) 3-	2.248e-010	1.954e-010	-9.648	-9.709	-0.061
S-2	6.644e-011	3.856e-011	-10.178	-10.414	-0.236
S (6)	1.978e-003				
SO4-2	1.500e-003	8.687e-004	-2.824	-3.061	-0.237
CaSO4	3.334e-004	3.349e-004	-3.477	-3.475	0.002
MgSO4	1.336e-004	1.343e-004	-3.874	-3.872	0.002
NaSO4-	9.015e-006	7.840e-006	-5.045	-5.106	-0.061
KSO4-	2.009e-006	1.747e-006	-5.697	-5.758	-0.061
MnSO4	2.755e-007	2.768e-007	-6.560	-6.558	0.002
FeSO4	2.681e-008	2.694e-008	-7.572	-7.570	0.002
HSO4-	6.876e-009	5.979e-009	-8.163	-8.223	-0.061
CaHSO4+	1.597e-010	1.389e-010	-9.797	-9.857	-0.061
FeHSO4+	1.442e-014	1.254e-014	-13.841	-13.902	-0.061
FeSO4+	4.185e-023	3.640e-023	-22.378	-22.439	-0.061
Fe (SO4) 2-	7.954e-025	6.917e-025	-24.099	-24.160	-0.061
FeHSO4+2	1.207e-029	6.900e-030	-28.918	-29.161	-0.243

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH) 5]	-4.50	18.59	23.09	Fe2(OH) 5
[Fe3(OH) 7]	1.14	26.13	24.99	Fe3(OH) 7
[Fe3(OH) 8]	-12.48	29.64	42.12	Fe3(OH) 8
[Fe6(OH) 12] [CO3]	-25.49	32.86	58.35	Fe6(OH) 12 (CO3) 1
[Fe6(OH) 12] [SO4]	-25.47	34.91	60.38	Fe6(OH) 12 (SO4) 1
[Fe6(OH) 8] [Cl]	-20.13	23.43	43.56	Fe4(OH) 8 (Cl) 1
Anhydrite	-1.41	-5.78	-4.36	CaSO4
Aragonite	0.51	-7.82	-8.34	CaCO3
Brucite	-5.67	11.12	16.79	Mg (OH) 2
Calcite	0.65	-7.82	-8.48	CaCO3
CO2 (g)	-1.26	-2.73	-1.47	CO2
Dolomite	0.97	-16.12	-17.09	CaMg (CO3) 2
Epsomite	-4.10	-6.24	-2.14	MgSO4:7H2O
Fe (OH) 2 (1)	-5.40	7.54	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-6.35	7.54	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-6.86	-1.97	4.89	Fe (OH) 3
FeO	-6.05	7.54	13.59	FeO
FeS (pom)	-0.34	-4.25	-3.91	FeS
FeS (ppt)	-0.34	-4.25	-3.92	FeS
Fluorite	-1.29	-11.89	-10.60	CaF2
Goethite	-0.97	-1.97	-1.00	FeOOH
Greigite	-4.81	-43.58	-38.77	Fe3S4
Gypsum	-1.19	-5.78	-4.58	CaSO4:2H2O
H2 (g)	-7.02	-10.17	-3.15	H2

H2O(g)	-1.51	-0.00	1.51	H2O
H2S(g)	-3.86	-4.85	-1.00	H2S
Halite	-7.42	-5.84	1.58	NaCl
Hausmannite	-28.35	32.68	61.03	Mn3O4
Hematite	0.07	-3.94	-4.01	Fe2O3
Jarosite-H3O	-28.52	-40.63	-12.11	H3OFe3(SO4)2(OH)6
Jarosite-K	-26.02	-37.02	-11.00	KFe3(SO4)2(OH)6
Lepidocrocite	-5.65	11.05	16.70	FeOOH
Lime	-11.22	11.59	22.81	Ca(OH)2
Mackinawite	0.39	-4.25	-4.64	FeS
Mackinawite(2)	-0.81	2.69	3.50	FeS
Magnetite	-16.15	29.65	45.80	Fe3O4
Manganite	-13.28	12.06	25.34	MnOOH
Marcasite	8.74	-9.03	-17.76	FeS2
Melanterite	-7.61	-9.82	-2.21	FeSO4·7H2O
Nesquehonite	-2.67	-8.29	-5.62	MgCO3·3H2O
O2(g)	-69.08	-72.04	-2.96	O2
Pyrite	9.45	-9.03	-18.48	FeS2
Pyrochroite	-6.65	8.55	15.20	Mn(OH)2
Pyrolusite	-25.81	15.57	41.38	MnO2
Rhodochrosite	0.27	-10.86	-11.13	MnCO3
Schwertmannite(1)	-57.50	-47.00	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-51.11	-33.11	18.00	Fe8O8(OH)6SO4
Siderite	-0.98	-11.87	-10.89	FeCO3
Sulfur	-2.71	2.17	4.88	S
Troilite	1.91	-4.25	-6.16	FeS

End of simulation.

Reading input data for simulation 2.

SOLUTION 1 TEMP-1 1-10-08 (In Biowall A)

temp	25
pH	6.35
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	29
F	0.56
S(6)	180 as SO4
S(-2)	1.9 as S
N(5)	0.5
N(3)	0.93
Ca	170
Fe	13
Mg	18
Mn	8.5
K	4.3
Na	24

Alkalinity 510 as HCO3
water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. TEMP-1 1-10-08 (In Biowall A)

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	8.358e-003	8.358e-003
Ca	4.242e-003	4.242e-003
Cl	8.180e-004	8.180e-004
F	2.948e-005	2.948e-005
Fe	2.328e-004	2.328e-004
K	1.100e-004	1.100e-004
Mg	7.404e-004	7.404e-004
Mn	1.547e-004	1.547e-004
N(3)	6.640e-005	6.640e-005
N(5)	3.570e-005	3.570e-005
Na	1.044e-003	1.044e-003
S(-2)	5.926e-005	5.926e-005
S(6)	1.874e-003	1.874e-003

-----Description of solution-----

pH	=	6.350
pe	=	4.000
Activity of water	=	1.000
Ionic strength	=	1.702e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	1.532e-002
Total CO2 (mol/kg)	=	1.532e-002
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	-1.162e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	-5.23
Iterations	=	9
Total H	=	1.110208e+002
Total O	=	5.555290e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
N(3)/N(5)	7.8003	0.4614
S(-2)/S(6)	-2.6844	-0.1588

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
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H+	4.988e-007	4.467e-007	-6.302	-6.350	-0.048
OH-	2.559e-008	2.240e-008	-7.592	-7.650	-0.058
H2O	5.551e+001	9.996e-001	1.744	-0.000	0.000
C (4)	1.532e-002				
HCO3-	7.929e-003	7.002e-003	-2.101	-2.155	-0.054
CO2	7.008e-003	7.035e-003	-2.154	-2.153	0.002
CaHCO3+	2.240e-004	1.979e-004	-3.650	-3.704	-0.054
FeHCO3+	6.714e-005	5.900e-005	-4.173	-4.229	-0.056
MnHCO3+	4.312e-005	3.789e-005	-4.365	-4.422	-0.056
MgHCO3+	3.594e-005	3.158e-005	-4.444	-4.501	-0.056
NaHCO3	3.576e-006	3.590e-006	-5.447	-5.445	0.002
MnCO3	3.531e-006	3.545e-006	-5.452	-5.450	0.002
CaCO3	2.725e-006	2.735e-006	-5.565	-5.563	0.002
FeCO3	1.480e-006	1.486e-006	-5.830	-5.828	0.002
CO3-2	1.208e-006	7.352e-007	-5.918	-6.134	-0.216
MgCO3	2.693e-007	2.704e-007	-6.570	-6.568	0.002
Fe (CO3) (OH) -	1.472e-008	1.294e-008	-7.832	-7.888	-0.056
NaCO3-	1.421e-008	1.248e-008	-7.848	-7.904	-0.056
Fe (CO3) 2-2	2.153e-009	1.283e-009	-8.667	-8.892	-0.225
Ca	4.242e-003				
Ca+2	3.643e-003	2.215e-003	-2.439	-2.655	-0.216
CaSO4	3.716e-004	3.730e-004	-3.430	-3.428	0.002
CaHCO3+	2.240e-004	1.979e-004	-3.650	-3.704	-0.054
CaCO3	2.725e-006	2.735e-006	-5.565	-5.563	0.002
CaF+	5.411e-007	4.755e-007	-6.267	-6.323	-0.056
CaHSO4+	1.111e-009	9.761e-010	-8.954	-9.010	-0.056
CaOH+	9.361e-010	8.226e-010	-9.029	-9.085	-0.056
Cl	8.180e-004				
Cl-	8.177e-004	7.162e-004	-3.087	-3.145	-0.058
MnCl+	2.016e-007	1.771e-007	-6.696	-6.752	-0.056
FeCl+	9.481e-008	8.330e-008	-7.023	-7.079	-0.056
MnCl2	5.516e-011	5.538e-011	-10.258	-10.257	0.002
MnCl3-	1.243e-014	1.093e-014	-13.905	-13.962	-0.056
FeCl+2	6.038e-022	3.599e-022	-21.219	-21.444	-0.225
FeCl2+	1.311e-024	1.152e-024	-23.883	-23.939	-0.056
FeCl3	8.216e-029	8.248e-029	-28.085	-28.084	0.002
F	2.948e-005				
F-	2.816e-005	2.465e-005	-4.550	-4.608	-0.058
MgF+	7.143e-007	6.276e-007	-6.146	-6.202	-0.056
CaF+	5.411e-007	4.755e-007	-6.267	-6.323	-0.056
FeF+	2.364e-008	2.077e-008	-7.626	-7.683	-0.056
HF	1.645e-008	1.651e-008	-7.784	-7.782	0.002
NaF	1.288e-008	1.293e-008	-7.890	-7.888	0.002
MnF+	1.178e-008	1.035e-008	-7.929	-7.985	-0.056
HF2-	1.777e-012	1.562e-012	-11.750	-11.806	-0.056
FeF+2	1.091e-018	6.501e-019	-17.962	-18.187	-0.225
FeF2+	7.260e-019	6.379e-019	-18.139	-18.195	-0.056
FeF3	2.482e-020	2.492e-020	-19.605	-19.603	0.002
Fe (2)	2.328e-004				
Fe+2	1.371e-004	8.426e-005	-3.863	-4.074	-0.211
FeHCO3+	6.714e-005	5.900e-005	-4.173	-4.229	-0.056
FeSO4	1.260e-005	1.265e-005	-4.900	-4.898	0.002
FeS	9.473e-006	9.511e-006	-5.023	-5.022	0.002

Fe (HS) 2	4.777e-006	4.795e-006	-5.321	-5.319	0.002
FeCO3	1.480e-006	1.486e-006	-5.830	-5.828	0.002
FeCl+	9.481e-008	8.330e-008	-7.023	-7.079	-0.056
FeOH+	6.786e-008	5.963e-008	-7.168	-7.225	-0.056
FeF+	2.364e-008	2.077e-008	-7.626	-7.683	-0.056
Fe (CO3) (OH) -	1.472e-008	1.294e-008	-7.832	-7.888	-0.056
Fe (HS) 3-	4.749e-009	4.173e-009	-8.323	-8.380	-0.056
Fe (CO3) 2-2	2.153e-009	1.283e-009	-8.667	-8.892	-0.225
FeHSO4+	4.226e-011	3.713e-011	-10.374	-10.430	-0.056
Fe (OH) 2	1.032e-012	1.036e-012	-11.986	-11.985	0.002
Fe (3)	2.544e-013				
Fe (OH) 2+	2.028e-013	1.782e-013	-12.693	-12.749	-0.056
Fe (OH) 3	5.116e-014	5.136e-014	-13.291	-13.289	0.002
FeOH+2	4.033e-016	2.404e-016	-15.394	-15.619	-0.225
Fe (OH) 4-	1.193e-016	1.048e-016	-15.923	-15.980	-0.056
FeF+2	1.091e-018	6.501e-019	-17.962	-18.187	-0.225
FeF2+	7.260e-019	6.379e-019	-18.139	-18.195	-0.056
FeSO4+	1.753e-019	1.540e-019	-18.756	-18.812	-0.056
Fe+3	4.495e-020	1.664e-020	-19.347	-19.779	-0.432
FeF3	2.482e-020	2.492e-020	-19.605	-19.603	0.002
Fe (SO4) 2-	3.237e-021	2.844e-021	-20.490	-20.546	-0.056
FeCl+2	6.038e-022	3.599e-022	-21.219	-21.444	-0.225
FeCl2+	1.311e-024	1.152e-024	-23.883	-23.939	-0.056
FeHSO4+2	3.090e-025	1.842e-025	-24.510	-24.735	-0.225
FeCl3	8.216e-029	8.248e-029	-28.085	-28.084	0.002
Fe2 (OH) 2+4	1.232e-029	1.556e-030	-28.909	-29.808	-0.899
Fe3 (OH) 4+5	1.469e-039	0.000e+000	-38.833	-40.237	-1.404
H (0)	6.580e-011				
H2	3.290e-011	3.303e-011	-10.483	-10.481	0.002
K	1.100e-004				
K+	1.093e-004	9.576e-005	-3.961	-4.019	-0.058
KSO4-	6.464e-007	5.680e-007	-6.190	-6.246	-0.056
KOH	7.401e-013	7.430e-013	-12.131	-12.129	0.002
Mg	7.404e-004				
Mg+2	6.275e-004	3.854e-004	-3.202	-3.414	-0.212
MgSO4	7.596e-005	7.626e-005	-4.119	-4.118	0.002
MgHCO3+	3.594e-005	3.158e-005	-4.444	-4.501	-0.056
MgF+	7.143e-007	6.276e-007	-6.146	-6.202	-0.056
MgCO3	2.693e-007	2.704e-007	-6.570	-6.568	0.002
MgOH+	1.538e-009	1.351e-009	-8.813	-8.869	-0.056
Mn (2)	1.547e-004				
Mn+2	9.878e-005	6.071e-005	-4.005	-4.217	-0.211
MnHCO3+	4.312e-005	3.789e-005	-4.365	-4.422	-0.056
MnSO4	9.077e-006	9.112e-006	-5.042	-5.040	0.002
MnCO3	3.531e-006	3.545e-006	-5.452	-5.450	0.002
MnCl+	2.016e-007	1.771e-007	-6.696	-6.752	-0.056
MnF+	1.178e-008	1.035e-008	-7.929	-7.985	-0.056
MnOH+	3.974e-009	3.492e-009	-8.401	-8.457	-0.056
MnCl2	5.516e-011	5.538e-011	-10.258	-10.257	0.002
Mn (NO3) 2	2.339e-013	2.348e-013	-12.631	-12.629	0.002
MnCl3-	1.243e-014	1.093e-014	-13.905	-13.962	-0.056
Mn (3)	1.243e-032				
Mn+3	1.243e-032	3.880e-033	-31.906	-32.411	-0.506
N (3)	6.640e-005				

NO2-	6.640e-005	5.798e-005	-4.178	-4.237	-0.059
N (5)	3.570e-005				
NO3-	3.570e-005	3.117e-005	-4.447	-4.506	-0.059
Mn (NO3) 2	2.339e-013	2.348e-013	-12.631	-12.629	0.002
Na	1.044e-003				
Na+	1.036e-003	9.118e-004	-2.985	-3.040	-0.055
NaSO4-	4.390e-006	3.857e-006	-5.358	-5.414	-0.056
NaHCO3	3.576e-006	3.590e-006	-5.447	-5.445	0.002
NaCO3-	1.421e-008	1.248e-008	-7.848	-7.904	-0.056
NaF	1.288e-008	1.293e-008	-7.890	-7.888	0.002
NaOH	1.343e-011	1.348e-011	-10.872	-10.870	0.002
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-71.420	-71.418	0.002
S (-2)	5.926e-005				
H2S	3.109e-005	3.121e-005	-4.507	-4.506	0.002
FeS	9.473e-006	9.511e-006	-5.023	-5.022	0.002
HS-	9.128e-006	7.991e-006	-5.040	-5.097	-0.058
Fe (HS) 2	4.777e-006	4.795e-006	-5.321	-5.319	0.002
Fe (HS) 3-	4.749e-009	4.173e-009	-8.323	-8.380	-0.056
S-2	3.577e-012	2.161e-012	-11.447	-11.665	-0.219
S (6)	1.874e-003				
SO4-2	1.399e-003	8.441e-004	-2.854	-3.074	-0.220
CaSO4	3.716e-004	3.730e-004	-3.430	-3.428	0.002
MgSO4	7.596e-005	7.626e-005	-4.119	-4.118	0.002
FeSO4	1.260e-005	1.265e-005	-4.900	-4.898	0.002
MnSO4	9.077e-006	9.112e-006	-5.042	-5.040	0.002
NaSO4-	4.390e-006	3.857e-006	-5.358	-5.414	-0.056
KSO4-	6.464e-007	5.680e-007	-6.190	-6.246	-0.056
HSO4-	4.172e-008	3.666e-008	-7.380	-7.436	-0.056
CaHSO4+	1.111e-009	9.761e-010	-8.954	-9.010	-0.056
FeHSO4+	4.226e-011	3.713e-011	-10.374	-10.430	-0.056
FeSO4+	1.753e-019	1.540e-019	-18.756	-18.812	-0.056
Fe (SO4) 2-	3.237e-021	2.844e-021	-20.490	-20.546	-0.056
FeHSO4+2	3.090e-025	1.842e-025	-24.510	-24.735	-0.225

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-2.17	20.92	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	4.55	29.54	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-8.91	33.21	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-18.10	40.25	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-17.07	43.31	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-14.89	28.67	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-1.37	-5.73	-4.36	CaSO4
Aragonite	-0.45	-8.79	-8.34	CaCO3
Brucite	-7.51	9.29	16.79	Mg (OH) 2
Calcite	-0.31	-8.79	-8.48	CaCO3
CO2 (g)	-0.68	-2.15	-1.47	CO2
Dolomite	-1.25	-18.34	-17.09	CaMg (CO3) 2
Epsomite	-4.35	-6.49	-2.14	MgSO4 : 7H2O
Fe (OH) 2 (1)	-4.31	8.63	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-5.26	8.63	13.89	Fe (OH) 2

Fe (OH) 3 (a)	-5.62	-0.73	4.89	Fe (OH) 3
FeO	-4.96	8.63	13.59	FeO
FeS (pom)	1.09	-2.82	-3.91	FeS
FeS (ppt)	1.09	-2.82	-3.92	FeS
Fluorite	-1.27	-11.87	-10.60	CaF2
Goethite	0.27	-0.73	-1.00	FeOOH
Greigite	0.15	-38.62	-38.77	Fe3S4
Gypsum	-1.15	-5.73	-4.58	CaSO4:2H2O
H2 (g)	-7.33	-10.48	-3.15	H2
H2O (g)	-1.51	-0.00	1.51	H2O
H2S (g)	-3.51	-4.51	-1.00	H2S
Halite	-7.77	-6.19	1.58	NaCl
Hausmannite	-28.25	32.78	61.03	Mn3O4
Hematite	2.55	-1.46	-4.01	Fe2O3
Jarosite-H3O	-21.62	-33.73	-12.11	H3OFe3 (SO4) 2 (OH) 6
Jarosite-K	-20.40	-31.40	-11.00	KFe3 (SO4) 2 (OH) 6
Lepidocrocite	-4.41	12.29	16.70	FeOOH
Lime	-12.77	10.04	22.81	Ca (OH) 2
Mackinawite	1.82	-2.82	-4.64	FeS
Mackinawite(2)	0.62	4.12	3.50	FeS
Magnetite	-12.59	33.21	45.80	Fe3O4
Manganite	-13.19	12.15	25.34	MnOOH
Marcasite	10.83	-6.94	-17.76	FeS2
Melanterite	-4.94	-7.15	-2.21	FeSO4:7H2O
Nesquehonite	-3.93	-9.55	-5.62	MgCO3:3H2O
O2 (g)	-68.46	-71.42	-2.96	O2
Pyrite	11.54	-6.94	-18.48	FeS2
Pyrochroite	-6.72	8.48	15.20	Mn (OH) 2
Pyrolusite	-25.57	15.81	41.38	MnO2
Rhodochrosite	0.78	-10.35	-11.13	MnCO3
Schwertmannite(1)	-44.73	-34.23	10.50	Fe8O8 (OH) 4.4 (SO4) 1.8:8.4H2O
Schwertmannite(2)	-39.61	-21.61	18.00	Fe8O8 (OH) 6SO4
Siderite	0.68	-10.21	-10.89	FeCO3
Sulfur	-2.06	2.83	4.88	S
Troilite	3.34	-2.82	-6.16	FeS

End of simulation.

Reading input data for simulation 3.

SOLUTION 1 MWT-26 1-10-08 (Upgradient of Biowalls B1/B2)

temp	25
pH	7.46
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	55
F	0.9
S(6)	1000 as SO4

S(-2) 1.0 as S
 N(5) 1.4
 N(3) 0.25
 Ca 230
 Fe 0.042
 Mg 49
 Mn 0.01
 K 26
 Na 120
 Alkalinity 476 as HCO3
 water 1 # kg

END

 Beginning of initial solution calculations.

Initial solution 1. MWT-26 1-10-08 (Upgradient of Biowalls B1/B2)

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	7.801e-003	7.801e-003
Ca	5.739e-003	5.739e-003
Cl	1.551e-003	1.551e-003
F	4.737e-005	4.737e-005
Fe	7.521e-007	7.521e-007
K	6.649e-004	6.649e-004
Mg	2.015e-003	2.015e-003
Mn	1.820e-007	1.820e-007
N(3)	1.785e-005	1.785e-005
N(5)	9.995e-005	9.995e-005
Na	5.220e-003	5.220e-003
S(-2)	3.119e-005	3.119e-005
S(6)	1.041e-002	1.041e-002

-----Description of solution-----

pH	=	7.460
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	3.399e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	8.211e-003
Total CO2 (mol/kg)	=	8.211e-003
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	-8.942e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	-21.49
Iterations	=	8
Total H	=	1.110201e+002
Total O	=	5.557234e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
N(3)/N(5)	7.1992	0.4259
S(-2)/S(6)	-3.8986	-0.2306

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.449e-007	2.886e-007	-6.462	-6.540	-0.077
H+	3.988e-008	3.467e-008	-7.399	-7.460	-0.061
H2O	5.551e+001	9.995e-001	1.744	-0.000	0.000
C(4)	8.211e-003				
HCO3-	7.406e-003	6.293e-003	-2.130	-2.201	-0.071
CO2	4.870e-004	4.908e-004	-3.312	-3.309	0.003
CaHCO3+	1.910e-004	1.623e-004	-3.719	-3.790	-0.071
MgHCO3+	5.995e-005	5.055e-005	-4.222	-4.296	-0.074
CaCO3	2.868e-005	2.891e-005	-4.542	-4.539	0.003
CO3-2	1.633e-005	8.511e-006	-4.787	-5.070	-0.283
NaHCO3	1.513e-005	1.525e-005	-4.820	-4.817	0.003
MgCO3	5.532e-006	5.576e-006	-5.257	-5.254	0.003
NaCO3-	8.100e-007	6.829e-007	-6.092	-6.166	-0.074
FeHCO3+	7.300e-008	6.155e-008	-7.137	-7.211	-0.074
MnCO3	3.089e-008	3.113e-008	-7.510	-7.507	0.003
MnHCO3+	3.063e-008	2.583e-008	-7.514	-7.588	-0.074
FeCO3	1.981e-008	1.997e-008	-7.703	-7.700	0.003
Fe(CO3)(OH)-	2.656e-009	2.239e-009	-8.576	-8.650	-0.074
Fe(CO3)2-2	3.951e-010	1.997e-010	-9.403	-9.700	-0.296
Ca	5.739e-003				
Ca+2	3.877e-003	2.022e-003	-2.412	-2.694	-0.283
CaSO4	1.641e-003	1.654e-003	-2.785	-2.781	0.003
CaHCO3+	1.910e-004	1.623e-004	-3.719	-3.790	-0.071
CaCO3	2.868e-005	2.891e-005	-4.542	-4.539	0.003
CaF+	7.775e-007	6.556e-007	-6.109	-6.183	-0.074
CaOH+	1.147e-008	9.672e-009	-7.940	-8.014	-0.074
CaHSO4+	3.985e-010	3.360e-010	-9.400	-9.474	-0.074
Cl	1.551e-003				
Cl-	1.551e-003	1.299e-003	-2.809	-2.886	-0.077
MnCl+	2.891e-010	2.438e-010	-9.539	-9.613	-0.074
FeCl+	2.081e-010	1.754e-010	-9.682	-9.756	-0.074
MnCl2	1.372e-013	1.383e-013	-12.863	-12.859	0.003
MnCl3-	5.869e-017	4.948e-017	-16.231	-16.306	-0.074
FeCl+2	9.159e-026	4.629e-026	-25.038	-25.334	-0.296
FeCl2+	3.187e-028	2.687e-028	-27.497	-27.571	-0.074
FeCl3	3.464e-032	3.491e-032	-31.460	-31.457	0.003
F	4.737e-005				
F-	4.450e-005	3.723e-005	-4.352	-4.429	-0.077
MgF+	2.003e-006	1.689e-006	-5.698	-5.772	-0.074
CaF+	7.775e-007	6.556e-007	-6.109	-6.183	-0.074
NaF	9.160e-008	9.232e-008	-7.038	-7.035	0.003
HF	1.921e-009	1.936e-009	-8.717	-8.713	0.003
FeF+	4.319e-011	3.641e-011	-10.365	-10.439	-0.074
MnF+	1.407e-011	1.186e-011	-10.852	-10.926	-0.074

HF2-	3.280e-013	2.765e-013	-12.484	-12.558	-0.074
FeF+2	1.377e-022	6.960e-023	-21.861	-22.157	-0.296
FeF2+	1.223e-022	1.032e-022	-21.912	-21.986	-0.074
FeF3	6.039e-024	6.087e-024	-23.219	-23.216	0.003
Fe (2)	7.521e-007				
FeS	3.630e-007	3.659e-007	-6.440	-6.437	0.003
Fe+2	1.845e-007	9.782e-008	-6.734	-7.010	-0.276
FeHCO3+	7.300e-008	6.155e-008	-7.137	-7.211	-0.074
FeSO4	7.077e-008	7.133e-008	-7.150	-7.147	0.003
Fe (HS) 2	3.654e-008	3.683e-008	-7.437	-7.434	0.003
FeCO3	1.981e-008	1.997e-008	-7.703	-7.700	0.003
Fe (CO3) (OH) -	2.656e-009	2.239e-009	-8.576	-8.650	-0.074
FeOH+	1.057e-009	8.916e-010	-8.976	-9.050	-0.074
Fe (CO3) 2-2	3.951e-010	1.997e-010	-9.403	-9.700	-0.296
FeCl+	2.081e-010	1.754e-010	-9.682	-9.756	-0.074
Fe (HS) 3-	9.777e-011	8.243e-011	-10.010	-10.084	-0.074
FeF+	4.319e-011	3.641e-011	-10.365	-10.439	-0.074
Fe (OH) 2	1.979e-013	1.995e-013	-12.703	-12.700	0.003
FeHSO4+	1.928e-014	1.626e-014	-13.715	-13.789	-0.074
Fe (3)	1.045e-014				
Fe (OH) 3	7.721e-015	7.782e-015	-14.112	-14.109	0.003
Fe (OH) 2+	2.485e-015	2.096e-015	-14.605	-14.679	-0.074
Fe (OH) 4-	2.426e-016	2.046e-016	-15.615	-15.689	-0.074
FeOH+2	4.344e-019	2.196e-019	-18.362	-18.658	-0.296
FeF+2	1.377e-022	6.960e-023	-21.861	-22.157	-0.296
FeF2+	1.223e-022	1.032e-022	-21.912	-21.986	-0.074
FeSO4+	6.291e-023	5.304e-023	-22.201	-22.275	-0.074
FeF3	6.039e-024	6.087e-024	-23.219	-23.216	0.003
Fe (SO4) 2-	5.644e-024	4.759e-024	-23.248	-23.323	-0.074
Fe+3	4.157e-024	1.180e-024	-23.381	-23.928	-0.547
FeCl+2	9.159e-026	4.629e-026	-25.038	-25.334	-0.296
FeCl2+	3.187e-028	2.687e-028	-27.497	-27.571	-0.074
FeHSO4+2	9.744e-030	4.925e-030	-29.011	-29.308	-0.296
FeCl3	3.464e-032	3.491e-032	-31.460	-31.457	0.003
Fe2 (OH) 2+4	1.988e-035	1.297e-036	-34.702	-35.887	-1.185
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-46.394	-48.246	-1.852
H (0)	1.059e-010				
H2	5.295e-011	5.337e-011	-10.276	-10.273	0.003
K	6.649e-004				
K+	6.464e-004	5.414e-004	-3.189	-3.266	-0.077
KSO4-	1.850e-005	1.560e-005	-4.733	-4.807	-0.074
KOH	5.369e-011	5.412e-011	-10.270	-10.267	0.003
Mg	2.015e-003				
Mg+2	1.293e-003	6.865e-004	-2.888	-3.163	-0.275
MgSO4	6.548e-004	6.600e-004	-3.184	-3.180	0.003
MgHCO3+	5.995e-005	5.055e-005	-4.222	-4.296	-0.074
MgCO3	5.532e-006	5.576e-006	-5.257	-5.254	0.003
MgF+	2.003e-006	1.689e-006	-5.698	-5.772	-0.074
MgOH+	3.677e-008	3.101e-008	-7.434	-7.509	-0.074
Mn (2)	1.820e-007				
Mn+2	8.684e-008	4.605e-008	-7.061	-7.337	-0.276
MnSO4	3.332e-008	3.358e-008	-7.477	-7.474	0.003
MnCO3	3.089e-008	3.113e-008	-7.510	-7.507	0.003
MnHCO3+	3.063e-008	2.583e-008	-7.514	-7.588	-0.074

MnCl+	2.891e-010	2.438e-010	-9.539	-9.613	-0.074
MnOH+	4.046e-011	3.412e-011	-10.393	-10.467	-0.074
MnF+	1.407e-011	1.186e-011	-10.852	-10.926	-0.074
MnCl2	1.372e-013	1.383e-013	-12.863	-12.859	0.003
Mn(NO3)2	1.260e-015	1.270e-015	-14.900	-14.896	0.003
MnCl3-	5.869e-017	4.948e-017	-16.231	-16.306	-0.074
Mn(3)	8.343e-037				
Mn+3	8.343e-037	1.797e-037	-36.079	-36.745	-0.667
N(3)	1.785e-005				
NO2-	1.785e-005	1.486e-005	-4.748	-4.828	-0.079
N(5)	9.995e-005				
NO3-	9.995e-005	8.324e-005	-4.000	-4.080	-0.079
Mn(NO3)2	1.260e-015	1.270e-015	-14.900	-14.896	0.003
Na	5.220e-003				
Na+	5.099e-003	4.309e-003	-2.293	-2.366	-0.073
NaSO4-	1.050e-004	8.857e-005	-3.979	-4.053	-0.074
NaHCO3	1.513e-005	1.525e-005	-4.820	-4.817	0.003
NaCO3-	8.100e-007	6.829e-007	-6.092	-6.166	-0.074
NaF	9.160e-008	9.232e-008	-7.038	-7.035	0.003
NaOH	8.143e-010	8.207e-010	-9.089	-9.086	0.003
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-71.838	-71.835	0.003
S(-2)	3.119e-005				
HS-	2.457e-005	2.055e-005	-4.610	-4.687	-0.077
H2S	6.183e-006	6.231e-006	-5.209	-5.205	0.003
FeS	3.630e-007	3.659e-007	-6.440	-6.437	0.003
Fe(HS)2	3.654e-008	3.683e-008	-7.437	-7.434	0.003
S-2	1.391e-010	7.160e-011	-9.857	-10.145	-0.288
Fe(HS)3-	9.777e-011	8.243e-011	-10.010	-10.084	-0.074
S(6)	1.041e-002				
SO4-2	7.990e-003	4.101e-003	-2.097	-2.387	-0.290
CaSO4	1.641e-003	1.654e-003	-2.785	-2.781	0.003
MgSO4	6.548e-004	6.600e-004	-3.184	-3.180	0.003
NaSO4-	1.050e-004	8.857e-005	-3.979	-4.053	-0.074
KSO4-	1.850e-005	1.560e-005	-4.733	-4.807	-0.074
FeSO4	7.077e-008	7.133e-008	-7.150	-7.147	0.003
MnSO4	3.332e-008	3.358e-008	-7.477	-7.474	0.003
HSO4-	1.640e-008	1.382e-008	-7.785	-7.859	-0.074
CaHSO4+	3.985e-010	3.360e-010	-9.400	-9.474	-0.074
FeHSO4+	1.928e-014	1.626e-014	-13.715	-13.789	-0.074
FeSO4+	6.291e-023	5.304e-023	-22.201	-22.275	-0.074
Fe(SO4)2-	5.644e-024	4.759e-024	-23.248	-23.323	-0.074
FeHSO4+2	9.744e-030	4.925e-030	-29.011	-29.308	-0.296

-----Saturation indices-----

Phase	SI log IAP		log KT	
[Fe2(OH)5]	-3.71	19.38	23.09	Fe2(OH)5
[Fe3(OH)7]	2.30	27.29	24.99	Fe3(OH)7
[Fe3(OH)8]	-11.27	30.85	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-23.76	34.59	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-23.10	37.28	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-18.71	24.85	43.56	Fe4(OH)8(Cl)1

Anhydrite	-0.72	-5.08	-4.36	CaSO4
Aragonite	0.57	-7.76	-8.34	CaCO3
Brucite	-5.04	11.76	16.79	Mg (OH) 2
Calcite	0.72	-7.76	-8.48	CaCO3
CO2 (g)	-1.84	-3.31	-1.47	CO2
Dolomite	1.09	-16.00	-17.09	CaMg (CO3) 2
Epsomite	-3.41	-5.55	-2.14	MgSO4:7H2O
Fe (OH) 2 (1)	-5.03	7.91	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-5.98	7.91	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-6.44	-1.55	4.89	Fe (OH) 3
FeO	-5.68	7.91	13.59	FeO
FeS (pom)	-0.32	-4.24	-3.91	FeS
FeS (ppt)	-0.32	-4.24	-3.92	FeS
Fluorite	-0.95	-11.55	-10.60	CaF2
Goethite	-0.55	-1.55	-1.00	FeOOH
Greigite	-5.00	-43.77	-38.77	Fe3S4
Gypsum	-0.50	-5.08	-4.58	CaSO4:2H2O
H2 (g)	-7.12	-10.27	-3.15	H2
H2O (g)	-1.51	-0.00	1.51	H2O
H2S (g)	-4.21	-5.21	-1.00	H2S
Halite	-6.83	-5.25	1.58	NaCl
Hausmannite	-31.16	29.87	61.03	Mn3O4
Hematite	0.91	-3.10	-4.01	Fe2O3
Jarosite-H3O	-27.15	-39.26	-12.11	H3OFe3 (SO4) 2 (OH) 6
Jarosite-K	-24.07	-35.07	-11.00	KFe3 (SO4) 2 (OH) 6
Lepidocrocite	-5.23	11.47	16.70	FeOOH
Lime	-10.58	12.23	22.81	Ca (OH) 2
Mackinawite	0.41	-4.24	-4.64	FeS
Mackinawite (2)	-0.80	2.70	3.50	FeS
Magnetite	-14.95	30.85	45.80	Fe3O4
Manganite	-14.20	11.14	25.34	MnOOH
Marcasite	8.50	-9.26	-17.76	FeS2
Melanterite	-7.19	-9.40	-2.21	FeSO4:7H2O
Nesquehonite	-2.61	-8.23	-5.62	MgCO3:3H2O
O2 (g)	-68.88	-71.84	-2.96	O2
Pyrite	9.22	-9.26	-18.48	FeS2
Pyrochroite	-7.62	7.58	15.20	Mn (OH) 2
Pyrolusite	-26.67	14.71	41.38	MnO2
Rhodochrosite	-1.28	-12.41	-11.13	MnCO3
Schwertmannite (1)	-54.04	-43.54	10.50	Fe8O8 (OH) 4.4 (SO4) 1.8:8.4H2O
Schwertmannite (2)	-47.70	-29.70	18.00	Fe8O8 (OH) 6SO4
Siderite	-1.19	-12.08	-10.89	FeCO3
Sulfur	-2.96	1.92	4.88	S
Troilite	1.93	-4.24	-6.16	FeS

End of simulation.

Reading input data for simulation 4.

SOLUTION 1 MWT-27 1-10-08 (Upgradient of Biowalls B1/B2)


```

temp      25
pH        6.46
pe        4
redox     S(-2)/S(6)
units     mg/kgw
density   1
Cl        40
F         1.1
S(6)      10 as SO4
S(-2)     0.6 as S
N(5)      0.98
N(3)      1.1
Ca        430
Fe        66
Mg        80
Mn        7.2
K         94
Na        50
water     1 # kg

```

END

Beginning of initial solution calculations.

Initial solution 1. MWT-27 1-10-08 (Upgradient of Biowalls B1/B2)

-----Solution composition-----

Elements	Molality	Moles
Ca	1.073e-002	1.073e-002
Cl	1.128e-003	1.128e-003
F	5.790e-005	5.790e-005
Fe	1.182e-003	1.182e-003
K	2.404e-003	2.404e-003
Mg	3.291e-003	3.291e-003
Mn	1.311e-004	1.311e-004
N(3)	7.853e-005	7.853e-005
N(5)	6.997e-005	6.997e-005
Na	2.175e-003	2.175e-003
S(-2)	1.871e-005	1.871e-005
S(6)	1.041e-004	1.041e-004

-----Description of solution-----

```

pH = 6.460
pe = 4.000
Activity of water = 1.000
Ionic strength = 3.359e-002
Mass of water (kg) = 1.000e+000
Total alkalinity (eq/kg) = 2.821e-005
Total carbon (mol/kg) = 0.000e+000
Total CO2 (mol/kg) = 0.000e+000
Temperature (deg C) = 25.000

```

Electrical balance (eq) = 3.367e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = 92.12
Iterations = 8
Total H = 1.110124e+002
Total O = 5.550700e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
N(3)/N(5)	7.8000	0.4614
S(-2)/S(6)	-2.8851	-0.1707

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	3.986e-007	3.467e-007	-6.399	-6.460	-0.061
OH-	3.447e-008	2.886e-008	-7.463	-7.540	-0.077
H2O	5.551e+001	9.996e-001	1.744	-0.000	0.000
Ca	1.073e-002				
Ca+2	1.069e-002	5.593e-003	-1.971	-2.252	-0.281
CaSO4	3.198e-005	3.223e-005	-4.495	-4.492	0.003
CaF+	2.391e-006	2.018e-006	-5.621	-5.695	-0.074
CaOH+	3.171e-009	2.676e-009	-8.499	-8.572	-0.074
CaHSO4+	7.759e-011	6.547e-011	-10.110	-10.184	-0.074
Cl	1.128e-003				
Cl-	1.127e-003	9.447e-004	-2.948	-3.025	-0.077
FeCl+	9.560e-007	8.067e-007	-6.020	-6.093	-0.074
MnCl+	3.161e-007	2.668e-007	-6.500	-6.574	-0.074
MnCl2	1.092e-010	1.100e-010	-9.962	-9.959	0.003
MnCl3-	3.392e-014	2.862e-014	-13.470	-13.543	-0.074
FeCl+2	4.332e-021	2.196e-021	-20.363	-20.658	-0.295
FeCl2+	1.098e-023	9.267e-024	-22.959	-23.033	-0.074
FeCl3	8.688e-028	8.755e-028	-27.061	-27.058	0.003
F	5.790e-005				
F-	4.947e-005	4.142e-005	-4.306	-4.383	-0.077
MgF+	5.651e-006	4.768e-006	-5.248	-5.322	-0.074
CaF+	2.391e-006	2.018e-006	-5.621	-5.695	-0.074
FeF+	3.036e-007	2.562e-007	-6.518	-6.591	-0.074
NaF	4.350e-008	4.384e-008	-7.362	-7.358	0.003
MnF+	2.354e-008	1.986e-008	-7.628	-7.702	-0.074
HF	2.137e-008	2.154e-008	-7.670	-7.667	0.003
HF2-	4.056e-012	3.423e-012	-11.392	-11.466	-0.074
FeF+2	9.966e-018	5.053e-018	-17.001	-17.296	-0.295
FeF2+	9.874e-018	8.331e-018	-17.006	-17.079	-0.074
FeF3	5.427e-019	5.469e-019	-18.265	-18.262	0.003
Fe(2)	1.182e-003				
Fe+2	1.163e-003	6.186e-004	-2.934	-3.209	-0.274
FeS	1.259e-005	1.268e-005	-4.900	-4.897	0.003
FeSO4	3.152e-006	3.177e-006	-5.501	-5.498	0.003
FeCl+	9.560e-007	8.067e-007	-6.020	-6.093	-0.074
Fe(HS)2	6.947e-007	7.001e-007	-6.158	-6.155	0.003

FeOH+	6.683e-007	5.640e-007	-6.175	-6.249	-0.074
FeF+	3.036e-007	2.562e-007	-6.518	-6.591	-0.074
Fe (HS) 3-	1.018e-010	8.591e-011	-9.992	-10.066	-0.074
Fe (OH) 2	1.252e-011	1.262e-011	-10.902	-10.899	0.003
FeHSO4+	8.581e-012	7.241e-012	-11.066	-11.140	-0.074
Fe (3)	2.129e-012				
Fe (OH) 2+	1.621e-012	1.368e-012	-11.790	-11.864	-0.074
Fe (OH) 3	5.041e-013	5.080e-013	-12.298	-12.294	0.003
FeOH+2	2.826e-015	1.433e-015	-14.549	-14.844	-0.295
Fe (OH) 4-	1.583e-015	1.336e-015	-14.801	-14.874	-0.074
FeF+2	9.966e-018	5.053e-018	-17.001	-17.296	-0.295
FeF2+	9.874e-018	8.331e-018	-17.006	-17.079	-0.074
FeF3	5.427e-019	5.469e-019	-18.265	-18.262	0.003
Fe+3	2.700e-019	7.697e-020	-18.569	-19.114	-0.545
FeSO4+	2.889e-020	2.437e-020	-19.539	-19.613	-0.074
FeCl+2	4.332e-021	2.196e-021	-20.363	-20.658	-0.295
Fe (SO4) 2-	1.825e-023	1.540e-023	-22.739	-22.812	-0.074
FeCl2+	1.098e-023	9.267e-024	-22.959	-23.033	-0.074
FeHSO4+2	4.464e-026	2.263e-026	-25.350	-25.645	-0.295
FeCl3	8.688e-028	8.755e-028	-27.061	-27.058	0.003
Fe2 (OH) 2+4	8.364e-028	5.525e-029	-27.078	-28.258	-1.180
Fe3 (OH) 4+5	1.102e-036	1.579e-038	-35.958	-37.802	-1.844
H (0)	9.950e-011				
H2	4.975e-011	5.014e-011	-10.303	-10.300	0.003
K	2.404e-003				
K+	2.403e-003	2.015e-003	-2.619	-2.696	-0.077
KSO4-	4.845e-007	4.089e-007	-6.315	-6.388	-0.074
KOH	1.999e-011	2.014e-011	-10.699	-10.696	0.003
Mg	3.291e-003				
Mg+2	3.273e-003	1.742e-003	-2.485	-2.759	-0.274
MgSO4	1.171e-005	1.180e-005	-4.932	-4.928	0.003
MgF+	5.651e-006	4.768e-006	-5.248	-5.322	-0.074
MgOH+	9.327e-009	7.870e-009	-8.030	-8.104	-0.074
Mn (2)	1.311e-004				
Mn+2	1.304e-004	6.931e-005	-3.885	-4.159	-0.274
MnSO4	3.532e-007	3.560e-007	-6.452	-6.449	0.003
MnCl+	3.161e-007	2.668e-007	-6.500	-6.574	-0.074
MnF+	2.354e-008	1.986e-008	-7.628	-7.702	-0.074
MnOH+	6.087e-009	5.136e-009	-8.216	-8.289	-0.074
MnCl2	1.092e-010	1.100e-010	-9.962	-9.959	0.003
Mn (NO3) 2	9.313e-013	9.385e-013	-12.031	-12.028	0.003
MnCl3-	3.392e-014	2.862e-014	-13.470	-13.543	-0.074
Mn (3)	1.287e-032				
Mn+3	1.287e-032	2.791e-033	-31.890	-32.554	-0.664
N (3)	7.853e-005				
NO2-	7.853e-005	6.546e-005	-4.105	-4.184	-0.079
N (5)	6.997e-005				
NO3-	6.997e-005	5.832e-005	-4.155	-4.234	-0.079
Mn (NO3) 2	9.313e-013	9.385e-013	-12.031	-12.028	0.003
Na	2.175e-003				
Na+	2.175e-003	1.839e-003	-2.663	-2.735	-0.073
NaSO4-	3.155e-007	2.662e-007	-6.501	-6.575	-0.074
NaF	4.350e-008	4.384e-008	-7.362	-7.358	0.003
NaOH	3.476e-011	3.503e-011	-10.459	-10.456	0.003

O(0)	0.000e+000					
O2	0.000e+000	0.000e+000	-71.784	-71.781	0.003	
S(-2)	1.871e-005					
FeS	1.259e-005	1.268e-005	-4.900	-4.897	0.003	
H2S	3.390e-006	3.416e-006	-5.470	-5.466	0.003	
HS-	1.346e-006	1.127e-006	-5.871	-5.948	-0.077	
Fe(HS)2	6.947e-007	7.001e-007	-6.158	-6.155	0.003	
Fe(HS)3-	1.018e-010	8.591e-011	-9.992	-10.066	-0.074	
S-2	7.602e-013	3.925e-013	-12.119	-12.406	-0.287	
S(6)	1.041e-004					
SO4-2	5.610e-005	2.888e-005	-4.251	-4.539	-0.288	
CaSO4	3.198e-005	3.223e-005	-4.495	-4.492	0.003	
MgSO4	1.171e-005	1.180e-005	-4.932	-4.928	0.003	
FeSO4	3.152e-006	3.177e-006	-5.501	-5.498	0.003	
KSO4-	4.845e-007	4.089e-007	-6.315	-6.388	-0.074	
MnSO4	3.532e-007	3.560e-007	-6.452	-6.449	0.003	
NaSO4-	3.155e-007	2.662e-007	-6.501	-6.575	-0.074	
HSO4-	1.154e-009	9.736e-010	-8.938	-9.012	-0.074	
CaHSO4+	7.759e-011	6.547e-011	-10.110	-10.184	-0.074	
FeHSO4+	8.581e-012	7.241e-012	-11.066	-11.140	-0.074	
FeSO4+	2.889e-020	2.437e-020	-19.539	-19.613	-0.074	
Fe(SO4)2-	1.825e-023	1.540e-023	-22.739	-22.812	-0.074	
FeHSO4+2	4.464e-026	2.263e-026	-25.350	-25.645	-0.295	

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH)5]	-0.09	23.00	23.09	Fe2(OH)5
[Fe3(OH)7]	7.72	32.71	24.99	Fe3(OH)7
[Fe3(OH)8]	-5.84	36.28	42.12	Fe3(OH)8
[Fe6(OH)12][SO4]	-12.42	47.96	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-10.63	32.93	43.56	Fe4(OH)8(Cl)1
Anhydrite	-2.43	-6.79	-4.36	CaSO4
Brucite	-6.63	10.16	16.79	Mg(OH)2
Epsomite	-5.16	-7.30	-2.14	MgSO4:7H2O
Fe(OH)2(1)	-3.23	9.71	12.94	Fe(OH)2
Fe(OH)2(2)	-4.18	9.71	13.89	Fe(OH)2
Fe(OH)3(a)	-4.63	0.27	4.89	Fe(OH)3
FeO	-3.88	9.71	13.59	FeO
FeS(pom)	1.22	-2.70	-3.91	FeS
FeS(ppt)	1.22	-2.70	-3.92	FeS
Fluorite	-0.42	-11.02	-10.60	CaF2
Goethite	1.27	0.27	-1.00	FeOOH
Greigite	-0.62	-39.39	-38.77	Fe3S4
Gypsum	-2.21	-6.79	-4.58	CaSO4:2H2O
H2(g)	-7.15	-10.30	-3.15	H2
H2O(g)	-1.51	-0.00	1.51	H2O
H2S(g)	-4.47	-5.47	-1.00	H2S
Halite	-7.34	-5.76	1.58	NaCl
Hausmannite	-27.60	33.43	61.03	Mn3O4
Hematite	4.54	0.53	-4.01	Fe2O3
Jarosite-H3O	-22.01	-34.12	-12.11	H3OFe3(SO4)2(OH)6
Jarosite-K	-19.36	-30.36	-11.00	KFe3(SO4)2(OH)6

Lepidocrocite	-3.41	13.29	16.70	FeOOH
Lime	-12.14	10.67	22.81	Ca (OH) 2
Mackinawite	1.95	-2.70	-4.64	FeS
Mackinawite(2)	0.74	4.24	3.50	FeS
Magnetite	-9.52	36.28	45.80	Fe3O4
Manganite	-13.00	12.34	25.34	MnOOH
Marcasite	9.81	-7.95	-17.76	FeS2
Melanterite	-5.54	-7.75	-2.21	FeSO4:7H2O
O2(g)	-68.82	-71.78	-2.96	O2
Pyrite	10.52	-7.95	-18.48	FeS2
Pyrochroite	-6.44	8.76	15.20	Mn (OH) 2
Pyrolusite	-25.47	15.91	41.38	MnO2
Schwertmannite(1)	-39.80	-29.30	10.50	Fe8O8 (OH) 4.4 (SO4) 1.8:8.4H2O
Schwertmannite(2)	-33.33	-15.33	18.00	Fe8O8 (OH) 6SO4
Sulfur	-3.20	1.68	4.88	S
Troilite	3.47	-2.70	-6.16	FeS

End of simulation.

Reading input data for simulation 5.

SOLUTION 1 MWT-28 1-10-08 (In Biowall B2)

temp	25
pH	6.35
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	9.2
F	0.62
S(6)	3.1 as SO4
S(-2)	1.6 as S
N(5)	1.0
N(3)	0.41
Ca	230
Fe	27
Mg	32
Mn	3.7
K	34
Na	16
Alkalinity	1950 as HCO3
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. MWT-28 1-10-08 (In Biowall B2)

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	3.196e-002	3.196e-002
Ca	5.739e-003	5.739e-003
Cl	2.595e-004	2.595e-004
F	3.263e-005	3.263e-005
Fe	4.835e-004	4.835e-004
K	8.695e-004	8.695e-004
Mg	1.316e-003	1.316e-003
Mn	6.735e-005	6.735e-005
N(3)	2.927e-005	2.927e-005
N(5)	7.139e-005	7.139e-005
Na	6.960e-004	6.960e-004
S(-2)	4.990e-005	4.990e-005
S(6)	3.227e-005	3.227e-005

-----Description of solution-----

pH	=	6.350
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	2.902e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	5.788e-002
Total CO2 (mol/kg)	=	5.788e-002
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	-1.564e-002
Percent error, 100*(Cat- An)/(Cat+ An)	=	-34.05
Iterations	=	10
Total H	=	1.110444e+002
Total O	=	5.565427e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
N(3)/N(5)	8.1289	0.4809
S(-2)/S(6)	-2.9022	-0.1717

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.102e-007	4.467e-007	-6.292	-6.350	-0.058
OH-	2.646e-008	2.239e-008	-7.577	-7.650	-0.073
H2O	5.551e+001	9.989e-001	1.744	-0.000	0.000
C(4)	5.788e-002				
HCO3-	3.032e-002	2.601e-002	-1.518	-1.585	-0.067
CO2	2.598e-002	2.615e-002	-1.585	-1.582	0.003
CaHCO3+	9.908e-004	8.498e-004	-3.004	-3.071	-0.067
FeHCO3+	2.909e-004	2.478e-004	-3.536	-3.606	-0.070
MgHCO3+	2.155e-004	1.835e-004	-3.667	-3.736	-0.070

MnHCO3+	3.851e-005	3.280e-005	-4.414	-4.484	-0.070
CaCO3	1.167e-005	1.175e-005	-4.933	-4.930	0.003
NaHCO3	8.526e-006	8.583e-006	-5.069	-5.066	0.003
FeCO3	6.199e-006	6.241e-006	-5.208	-5.205	0.003
CO3-2	5.045e-006	2.731e-006	-5.297	-5.564	-0.267
MnCO3	3.049e-006	3.069e-006	-5.516	-5.513	0.003
MgCO3	1.561e-006	1.571e-006	-5.807	-5.804	0.003
Fe (CO3) (OH) -	6.375e-008	5.429e-008	-7.196	-7.265	-0.070
Fe (CO3) 2-2	3.805e-008	2.002e-008	-7.420	-7.698	-0.279
NaCO3-	3.503e-008	2.984e-008	-7.456	-7.525	-0.070
Ca	5.739e-003				
Ca+2	4.729e-003	2.561e-003	-2.325	-2.592	-0.266
CaHCO3+	9.908e-004	8.498e-004	-3.004	-3.071	-0.067
CaCO3	1.167e-005	1.175e-005	-4.933	-4.930	0.003
CaSO4	6.425e-006	6.468e-006	-5.192	-5.189	0.003
CaF+	6.798e-007	5.790e-007	-6.168	-6.237	-0.070
CaOH+	1.116e-009	9.503e-010	-8.952	-9.022	-0.070
CaHSO4+	1.987e-011	1.693e-011	-10.702	-10.771	-0.070
Cl	2.595e-004				
Cl-	2.594e-004	2.198e-004	-3.586	-3.658	-0.072
FeCl+	3.393e-008	2.890e-008	-7.469	-7.539	-0.070
MnCl+	1.487e-008	1.267e-008	-7.828	-7.897	-0.070
MnCl2	1.207e-012	1.215e-012	-11.918	-11.915	0.003
MnCl3-	8.634e-017	7.354e-017	-16.064	-16.133	-0.070
FeCl+2	1.437e-022	7.563e-023	-21.843	-22.121	-0.279
FeCl2+	8.716e-026	7.423e-026	-25.060	-25.129	-0.070
FeCl3	1.620e-030	1.631e-030	-29.790	-29.787	0.003
F	3.263e-005				
F-	3.068e-005	2.596e-005	-4.513	-4.586	-0.073
MgF+	1.214e-006	1.034e-006	-5.916	-5.985	-0.070
CaF+	6.798e-007	5.790e-007	-6.168	-6.237	-0.070
FeF+	2.904e-008	2.473e-008	-7.537	-7.607	-0.070
HF	1.728e-008	1.739e-008	-7.763	-7.760	0.003
NaF	8.707e-009	8.766e-009	-8.060	-8.057	0.003
MnF+	2.984e-009	2.541e-009	-8.525	-8.595	-0.070
HF2-	2.034e-012	1.732e-012	-11.692	-11.761	-0.070
FeF+2	8.909e-019	4.689e-019	-18.050	-18.329	-0.279
FeF2+	5.690e-019	4.846e-019	-18.245	-18.315	-0.070
FeF3	1.981e-020	1.994e-020	-19.703	-19.700	0.003
Fe (2)	4.835e-004				
FeHCO3+	2.909e-004	2.478e-004	-3.536	-3.606	-0.070
Fe+2	1.733e-004	9.526e-005	-3.761	-4.021	-0.260
FeS	8.871e-006	8.931e-006	-5.052	-5.049	0.003
FeCO3	6.199e-006	6.241e-006	-5.208	-5.205	0.003
Fe (HS) 2	3.715e-006	3.740e-006	-5.430	-5.427	0.003
FeSO4	2.130e-007	2.145e-007	-6.672	-6.669	0.003
FeOH+	7.909e-008	6.737e-008	-7.102	-7.172	-0.070
Fe (CO3) (OH) -	6.375e-008	5.429e-008	-7.196	-7.265	-0.070
Fe (CO3) 2-2	3.805e-008	2.002e-008	-7.420	-7.698	-0.279
FeCl+	3.393e-008	2.890e-008	-7.469	-7.539	-0.070
FeF+	2.904e-008	2.473e-008	-7.537	-7.607	-0.070
Fe (HS) 3-	3.173e-009	2.703e-009	-8.499	-8.568	-0.070
Fe (OH) 2	1.162e-012	1.169e-012	-11.935	-11.932	0.003
FeHSO4+	7.393e-013	6.297e-013	-12.131	-12.201	-0.070

Fe (3)	1.783e-013					
Fe (OH) 2+	1.430e-013	1.218e-013	-12.845	-12.914	-0.070	
Fe (OH) 3	3.486e-014	3.510e-014	-13.458	-13.455	0.003	
FeOH+2	3.126e-016	1.645e-016	-15.505	-15.784	-0.279	
Fe (OH) 4-	8.404e-017	7.158e-017	-16.076	-16.145	-0.070	
FeF+2	8.909e-019	4.689e-019	-18.050	-18.329	-0.279	
FeF2+	5.690e-019	4.846e-019	-18.245	-18.315	-0.070	
Fe+3	3.768e-020	1.140e-020	-19.424	-19.943	-0.519	
FeF3	1.981e-020	1.994e-020	-19.703	-19.700	0.003	
FeSO4+	1.857e-021	1.582e-021	-20.731	-20.801	-0.070	
FeCl+2	1.437e-022	7.563e-023	-21.843	-22.121	-0.279	
Fe (SO4) 2-	5.144e-025	4.381e-025	-24.289	-24.358	-0.070	
FeCl2+	8.716e-026	7.423e-026	-25.060	-25.129	-0.070	
FeHSO4+2	3.595e-027	1.892e-027	-26.444	-26.723	-0.279	
Fe2 (OH) 2+4	9.497e-030	7.286e-031	-29.022	-30.138	-1.115	
FeCl3	1.620e-030	1.631e-030	-29.790	-29.787	0.003	
Fe3 (OH) 4+5	1.025e-039	0.000e+000	-38.989	-40.732	-1.742	
H (0)	1.789e-010					
H2	8.943e-011	9.003e-011	-10.049	-10.046	0.003	
K	8.695e-004					
K+	8.694e-004	7.364e-004	-3.061	-3.133	-0.072	
KSO4-	7.691e-008	6.551e-008	-7.114	-7.184	-0.070	
KOH	5.672e-012	5.710e-012	-11.246	-11.243	0.003	
Mg	1.316e-003					
Mg+2	1.096e-003	6.030e-004	-2.960	-3.220	-0.260	
MgHCO3+	2.155e-004	1.835e-004	-3.667	-3.736	-0.070	
MgSO4	1.778e-006	1.789e-006	-5.750	-5.747	0.003	
MgCO3	1.561e-006	1.571e-006	-5.807	-5.804	0.003	
MgF+	1.214e-006	1.034e-006	-5.916	-5.985	-0.070	
MgOH+	2.480e-009	2.113e-009	-8.605	-8.675	-0.070	
Mn (2)	6.735e-005					
MnHCO3+	3.851e-005	3.280e-005	-4.414	-4.484	-0.070	
Mn+2	2.574e-005	1.415e-005	-4.589	-4.849	-0.260	
MnCO3	3.049e-006	3.069e-006	-5.516	-5.513	0.003	
MnSO4	3.164e-008	3.185e-008	-7.500	-7.497	0.003	
MnCl+	1.487e-008	1.267e-008	-7.828	-7.897	-0.070	
MnF+	2.984e-009	2.541e-009	-8.525	-8.595	-0.070	
MnOH+	9.549e-010	8.133e-010	-9.020	-9.090	-0.070	
MnCl2	1.207e-012	1.215e-012	-11.918	-11.915	0.003	
Mn (NO3) 2	2.026e-013	2.039e-013	-12.693	-12.691	0.003	
MnCl3-	8.634e-017	7.354e-017	-16.064	-16.133	-0.070	
Mn (3)	2.322e-033					
Mn+3	2.322e-033	5.477e-034	-32.634	-33.261	-0.627	
N (3)	2.927e-005					
NO2-	2.927e-005	2.467e-005	-4.534	-4.608	-0.074	
N (5)	7.139e-005					
NO3-	7.139e-005	6.017e-005	-4.146	-4.221	-0.074	
Mn (NO3) 2	2.026e-013	2.039e-013	-12.693	-12.691	0.003	
Na	6.960e-004					
Na+	6.873e-004	5.868e-004	-3.163	-3.232	-0.069	
NaHCO3	8.526e-006	8.583e-006	-5.069	-5.066	0.003	
NaSO4-	4.371e-008	3.723e-008	-7.359	-7.429	-0.070	
NaCO3-	3.503e-008	2.984e-008	-7.456	-7.525	-0.070	
NaF	8.707e-009	8.766e-009	-8.060	-8.057	0.003	

NaOH	8.611e-012	8.669e-012	-11.065	-11.062	0.003
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-72.293	-72.290	0.003
S (-2)	4.990e-005				
H2S	2.575e-005	2.592e-005	-4.589	-4.586	0.003
FeS	8.871e-006	8.931e-006	-5.052	-5.049	0.003
HS-	7.843e-006	6.637e-006	-5.105	-5.178	-0.073
Fe (HS) 2	3.715e-006	3.740e-006	-5.430	-5.427	0.003
Fe (HS) 3-	3.173e-009	2.703e-009	-8.499	-8.568	-0.070
S-2	3.351e-012	1.795e-012	-11.475	-11.746	-0.271
S (6)	3.227e-005				
SO4-2	2.370e-005	1.266e-005	-4.625	-4.898	-0.272
CaSO4	6.425e-006	6.468e-006	-5.192	-5.189	0.003
MgSO4	1.778e-006	1.789e-006	-5.750	-5.747	0.003
FeSO4	2.130e-007	2.145e-007	-6.672	-6.669	0.003
KSO4-	7.691e-008	6.551e-008	-7.114	-7.184	-0.070
NaSO4-	4.371e-008	3.723e-008	-7.359	-7.429	-0.070
MnSO4	3.164e-008	3.185e-008	-7.500	-7.497	0.003
HSO4-	6.455e-010	5.498e-010	-9.190	-9.260	-0.070
CaHSO4+	1.987e-011	1.693e-011	-10.702	-10.771	-0.070
FeHSO4+	7.393e-013	6.297e-013	-12.131	-12.201	-0.070
FeSO4+	1.857e-021	1.582e-021	-20.731	-20.801	-0.070
Fe (SO4) 2-	5.144e-025	4.381e-025	-24.289	-24.358	-0.070
FeHSO4+2	3.595e-027	1.892e-027	-26.444	-26.723	-0.279

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-2.29	20.80	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	4.49	29.48	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-9.19	32.93	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-17.65	40.70	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-19.01	41.37	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-15.41	28.15	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-3.13	-7.49	-4.36	CaSO4
Aragonite	0.18	-8.16	-8.34	CaCO3
Brucite	-7.31	9.48	16.79	Mg (OH) 2
Calcite	0.32	-8.16	-8.48	CaCO3
CO2 (g)	-0.11	-1.58	-1.47	CO2
Dolomite	0.15	-16.94	-17.09	CaMg (CO3) 2
Epsomite	-5.98	-8.12	-2.14	MgSO4:7H2O
Fe (OH) 2 (1)	-4.26	8.68	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-5.21	8.68	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-5.79	-0.89	4.89	Fe (OH) 3
FeO	-4.91	8.68	13.59	FeO
FeS (pom)	1.06	-2.85	-3.91	FeS
FeS (ppt)	1.07	-2.85	-3.92	FeS
Fluorite	-1.16	-11.76	-10.60	CaF2
Goethite	0.11	-0.89	-1.00	FeOOH
Greigite	-0.45	-39.22	-38.77	Fe3S4
Gypsum	-2.91	-7.49	-4.58	CaSO4:2H2O
H2 (g)	-6.90	-10.05	-3.15	H2
H2O (g)	-1.51	-0.00	1.51	H2O

H2S(g)	-3.59	-4.59	-1.00	H2S
Halite	-8.47	-6.89	1.58	NaCl
Hausmannite	-30.58	30.45	61.03	Mn3O4
Hematite	2.22	-1.79	-4.01	Fe2O3
Jarosite-H3O	-25.77	-37.88	-12.11	H3OFe3(SO4)2(OH)6
Jarosite-K	-23.66	-34.66	-11.00	KFe3(SO4)2(OH)6
Lepidocrocite	-4.57	12.13	16.70	FeOOH
Lime	-12.70	10.11	22.81	Ca(OH)2
Mackinawite	1.79	-2.85	-4.64	FeS
Mackinawite(2)	0.59	4.09	3.50	FeS
Magnetite	-12.87	32.93	45.80	Fe3O4
Manganite	-14.04	11.30	25.34	MnOOH
Marcasite	10.28	-7.48	-17.76	FeS2
Melanterite	-6.71	-8.92	-2.21	FeSO4·7H2O
Nesquehonite	-3.16	-8.78	-5.62	MgCO3·3H2O
O2(g)	-69.33	-72.29	-2.96	O2
Pyrite	11.00	-7.48	-18.48	FeS2
Pyrochroite	-7.35	7.85	15.20	Mn(OH)2
Pyrolusite	-26.63	14.75	41.38	MnO2
Rhodochrosite	0.72	-10.41	-11.13	MnCO3
Schwertmannite(1)	-49.33	-38.83	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-42.75	-24.75	18.00	Fe8O8(OH)6SO4
Siderite	1.31	-9.58	-10.89	FeCO3
Sulfur	-2.57	2.31	4.88	S
Troilite	3.31	-2.85	-6.16	FeS

End of simulation.

Reading input data for simulation 6.

SOLUTION 1 MWT-29 1-10-08 (downgradient of Biowall B2)

temp	25
pH	6.70
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	18.0
F	0.74
S(6)	220 as SO4
S(-2)	1.0 as S
N(5)	1.3
N(3)	0.25
Ca	160
Fe	0.1
Mg	29
Mn	0.9
K	13
Na	44
Alkalinity	850 as HCO3

water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. MWT-29 1-10-08 (downgradient of Biowall B2)

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.393e-002	1.393e-002
Ca	3.992e-003	3.992e-003
Cl	5.077e-004	5.077e-004
F	3.895e-005	3.895e-005
Fe	1.791e-006	1.791e-006
K	3.325e-004	3.325e-004
Mg	1.193e-003	1.193e-003
Mn	1.638e-005	1.638e-005
N(3)	1.785e-005	1.785e-005
N(5)	9.281e-005	9.281e-005
Na	1.914e-003	1.914e-003
S(-2)	3.119e-005	3.119e-005
S(6)	2.290e-003	2.290e-003

-----Description of solution-----

pH	=	6.700
pe	=	4.000
Activity of water	=	1.000
Ionic strength	=	2.039e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	1.916e-002
Total CO2 (mol/kg)	=	1.916e-002
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	-6.515e-003
Percent error, 100*(Cat- An)/(Cat+ An)	=	-22.64
Iterations	=	9
Total H	=	1.110264e+002
Total O	=	5.556791e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
N(3)/N(5)	7.9431	0.4699
S(-2)/S(6)	-3.0838	-0.1824

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
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H+	2.245e-007	1.995e-007	-6.649	-6.700	-0.051
OH-	5.791e-008	5.015e-008	-7.237	-7.300	-0.062
H2O	5.551e+001	9.995e-001	1.744	-0.000	0.000
C (4)	1.916e-002				
HCO3-	1.345e-002	1.177e-002	-1.871	-1.929	-0.058
CO2	5.256e-003	5.281e-003	-2.279	-2.277	0.002
CaHCO3+	3.284e-004	2.873e-004	-3.484	-3.542	-0.058
MgHCO3+	9.041e-005	7.865e-005	-4.044	-4.104	-0.061
NaHCO3	1.087e-005	1.092e-005	-4.964	-4.962	0.002
CaCO3	8.850e-006	8.891e-006	-5.053	-5.051	0.002
MnHCO3+	5.996e-006	5.216e-006	-5.222	-5.283	-0.061
CO3-2	4.720e-006	2.766e-006	-5.326	-5.558	-0.232
MgCO3	1.501e-006	1.508e-006	-5.824	-5.822	0.002
MnCO3	1.088e-006	1.093e-006	-5.964	-5.961	0.002
FeHCO3+	6.496e-007	5.651e-007	-6.187	-6.248	-0.061
NaCO3-	9.768e-008	8.497e-008	-7.010	-7.071	-0.061
FeCO3	3.171e-008	3.186e-008	-7.499	-7.497	0.002
Fe (CO3) (OH) -	7.138e-010	6.209e-010	-9.146	-9.207	-0.061
Fe (CO3) 2-2	1.808e-010	1.035e-010	-9.743	-9.985	-0.242
Ca	3.992e-003				
Ca+2	3.267e-003	1.914e-003	-2.486	-2.718	-0.232
CaSO4	3.869e-004	3.887e-004	-3.412	-3.410	0.002
CaHCO3+	3.284e-004	2.873e-004	-3.484	-3.542	-0.058
CaCO3	8.850e-006	8.891e-006	-5.053	-5.051	0.002
CaF+	6.125e-007	5.328e-007	-6.213	-6.273	-0.061
CaOH+	1.829e-009	1.591e-009	-8.738	-8.798	-0.061
CaHSO4+	5.223e-010	4.543e-010	-9.282	-9.343	-0.061
Cl	5.077e-004				
Cl-	5.077e-004	4.400e-004	-3.294	-3.357	-0.062
MnCl+	1.025e-008	8.916e-009	-7.989	-8.050	-0.061
FeCl+	3.353e-010	2.917e-010	-9.475	-9.535	-0.061
MnCl2	1.704e-012	1.712e-012	-11.768	-11.766	0.002
MnCl3-	2.385e-016	2.075e-016	-15.622	-15.683	-0.061
FeCl+2	8.773e-025	5.024e-025	-24.057	-24.299	-0.242
FeCl2+	1.135e-027	9.874e-028	-26.945	-27.006	-0.061
FeCl3	4.324e-032	4.345e-032	-31.364	-31.362	0.002
F	3.895e-005				
F-	3.691e-005	3.196e-005	-4.433	-4.495	-0.062
MgF+	1.387e-006	1.206e-006	-5.858	-5.919	-0.061
CaF+	6.125e-007	5.328e-007	-6.213	-6.273	-0.061
NaF	3.021e-008	3.035e-008	-7.520	-7.518	0.002
HF	9.520e-009	9.565e-009	-8.021	-8.019	0.002
MnF+	1.264e-009	1.100e-009	-8.898	-8.959	-0.061
FeF+	1.765e-010	1.535e-010	-9.753	-9.814	-0.061
HF2-	1.349e-012	1.173e-012	-11.870	-11.931	-0.061
FeF+2	3.345e-021	1.916e-021	-20.476	-20.718	-0.242
FeF2+	2.802e-021	2.438e-021	-20.553	-20.613	-0.061
FeF3	1.229e-022	1.235e-022	-21.910	-21.908	0.002
Fe (2)	1.791e-006				
Fe+2	8.100e-007	4.802e-007	-6.092	-6.319	-0.227
FeHCO3+	6.496e-007	5.651e-007	-6.187	-6.248	-0.061
FeS	1.617e-007	1.625e-007	-6.791	-6.789	0.002
FeSO4	8.652e-008	8.693e-008	-7.063	-7.061	0.002
Fe (HS) 2	4.875e-008	4.898e-008	-7.312	-7.310	0.002

FeCO ₃	3.171e-008	3.186e-008	-7.499	-7.497	0.002
FeOH+	8.745e-010	7.608e-010	-9.058	-9.119	-0.061
Fe (CO ₃) (OH) -	7.138e-010	6.209e-010	-9.146	-9.207	-0.061
FeCl+	3.353e-010	2.917e-010	-9.475	-9.535	-0.061
Fe (CO ₃) 2-2	1.808e-010	1.035e-010	-9.743	-9.985	-0.242
FeF+	1.765e-010	1.535e-010	-9.753	-9.814	-0.061
Fe (HS) 3-	6.559e-011	5.706e-011	-10.183	-10.244	-0.061
FeHSO ₄ +	1.311e-013	1.140e-013	-12.883	-12.943	-0.061
Fe (OH) 2	2.944e-014	2.958e-014	-13.531	-13.529	0.002
Fe (3)	3.644e-015				
Fe (OH) 2+	2.332e-015	2.029e-015	-14.632	-14.693	-0.061
Fe (OH) 3	1.303e-015	1.309e-015	-14.885	-14.883	0.002
Fe (OH) 4-	6.875e-018	5.981e-018	-17.163	-17.223	-0.061
FeOH+2	2.135e-018	1.223e-018	-17.671	-17.913	-0.242
FeF+2	3.345e-021	1.916e-021	-20.476	-20.718	-0.242
FeF ₂ +	2.802e-021	2.438e-021	-20.553	-20.613	-0.061
FeSO ₄ +	4.851e-022	4.220e-022	-21.314	-21.375	-0.061
FeF ₃	1.229e-022	1.235e-022	-21.910	-21.908	0.002
Fe+3	1.091e-022	3.781e-023	-21.962	-22.422	-0.460
Fe (SO ₄) 2-	1.080e-023	9.397e-024	-22.966	-23.027	-0.061
FeCl+2	8.773e-025	5.024e-025	-24.057	-24.299	-0.242
FeCl ₂ +	1.135e-027	9.874e-028	-26.945	-27.006	-0.061
FeHSO ₄ +2	3.937e-028	2.255e-028	-27.405	-27.647	-0.242
FeCl ₃	4.324e-032	4.345e-032	-31.364	-31.362	0.002
Fe ₂ (OH) 2+4	3.742e-034	4.025e-035	-33.427	-34.395	-0.968
Fe ₃ (OH) 4+5	0.000e+000	0.000e+000	-45.255	-46.768	-1.513
H (0)	8.254e-011				
H ₂	4.127e-011	4.147e-011	-10.384	-10.382	0.002
K	3.325e-004				
K+	3.301e-004	2.861e-004	-3.481	-3.544	-0.062
KSO ₄ -	2.352e-006	2.046e-006	-5.629	-5.689	-0.061
KOH	4.946e-012	4.969e-012	-11.306	-11.304	0.002
Mg	1.193e-003				
Mg+2	9.639e-004	5.712e-004	-3.016	-3.243	-0.227
MgSO ₄	1.357e-004	1.363e-004	-3.868	-3.865	0.002
MgHCO ₃ +	9.041e-005	7.865e-005	-4.044	-4.104	-0.061
MgCO ₃	1.501e-006	1.508e-006	-5.824	-5.822	0.002
MgF+	1.387e-006	1.206e-006	-5.858	-5.919	-0.061
MgOH+	5.154e-009	4.483e-009	-8.288	-8.348	-0.061
Mn (2)	1.638e-005				
Mn+2	8.390e-006	4.974e-006	-5.076	-5.303	-0.227
MnHCO ₃ +	5.996e-006	5.216e-006	-5.222	-5.283	-0.061
MnCO ₃	1.088e-006	1.093e-006	-5.964	-5.961	0.002
MnSO ₄	8.961e-007	9.004e-007	-6.048	-6.046	0.002
MnCl+	1.025e-008	8.916e-009	-7.989	-8.050	-0.061
MnF+	1.264e-009	1.100e-009	-8.898	-8.959	-0.061
MnOH+	7.363e-010	6.405e-010	-9.133	-9.193	-0.061
MnCl ₂	1.704e-012	1.712e-012	-11.768	-11.766	0.002
Mn (NO ₃) 2	1.266e-013	1.272e-013	-12.898	-12.896	0.002
MnCl ₃ -	2.385e-016	2.075e-016	-15.622	-15.683	-0.061
Mn (3)	4.442e-034				
Mn+3	4.442e-034	1.267e-034	-33.352	-33.897	-0.545
N (3)	1.785e-005				
NO ₂ -	1.785e-005	1.541e-005	-4.748	-4.812	-0.064

N (5)	9.281e-005					
NO3-	9.281e-005	8.014e-005	-4.032	-4.096	-0.064	
Mn (NO3) 2	1.266e-013	1.272e-013	-12.898	-12.896	0.002	
Na	1.914e-003					
Na+	1.893e-003	1.650e-003	-2.723	-2.783	-0.060	
NaHCO3	1.087e-005	1.092e-005	-4.964	-4.962	0.002	
NaSO4-	9.676e-006	8.418e-006	-5.014	-5.075	-0.061	
NaCO3-	9.768e-008	8.497e-008	-7.010	-7.071	-0.061	
NaF	3.021e-008	3.035e-008	-7.520	-7.518	0.002	
NaOH	5.436e-011	5.461e-011	-10.265	-10.263	0.002	
O (0)	0.000e+000					
O2	0.000e+000	0.000e+000	-71.618	-71.616	0.002	
S (-2)	3.119e-005					
H2S	1.858e-005	1.866e-005	-4.731	-4.729	0.002	
HS-	1.235e-005	1.070e-005	-4.908	-4.971	-0.062	
FeS	1.617e-007	1.625e-007	-6.791	-6.789	0.002	
Fe (HS) 2	4.875e-008	4.898e-008	-7.312	-7.310	0.002	
Fe (HS) 3-	6.559e-011	5.706e-011	-10.183	-10.244	-0.061	
S-2	1.114e-011	6.476e-012	-10.953	-11.189	-0.236	
S (6)	2.290e-003					
SO4-2	1.755e-003	1.018e-003	-2.756	-2.992	-0.236	
CaSO4	3.869e-004	3.887e-004	-3.412	-3.410	0.002	
MgSO4	1.357e-004	1.363e-004	-3.868	-3.865	0.002	
NaSO4-	9.676e-006	8.418e-006	-5.014	-5.075	-0.061	
KSO4-	2.352e-006	2.046e-006	-5.629	-5.689	-0.061	
MnSO4	8.961e-007	9.004e-007	-6.048	-6.046	0.002	
FeSO4	8.652e-008	8.693e-008	-7.063	-7.061	0.002	
HSO4-	2.270e-008	1.975e-008	-7.644	-7.705	-0.061	
CaHSO4+	5.223e-010	4.543e-010	-9.282	-9.343	-0.061	
FeHSO4+	1.311e-013	1.140e-013	-12.883	-12.943	-0.061	
FeSO4+	4.851e-022	4.220e-022	-21.314	-21.375	-0.061	
Fe (SO4) 2-	1.080e-023	9.397e-024	-22.966	-23.027	-0.061	
FeHSO4+2	3.937e-028	2.255e-028	-27.405	-27.647	-0.242	

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-5.31	17.78	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	-0.13	24.86	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-13.65	28.47	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-27.59	30.76	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-27.05	33.33	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-21.68	21.88	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-1.35	-5.71	-4.36	CaSO4
Aragonite	0.06	-8.28	-8.34	CaCO3
Brucite	-6.64	10.16	16.79	Mg (OH) 2
Calcite	0.20	-8.28	-8.48	CaCO3
CO2 (g)	-0.81	-2.28	-1.47	CO2
Dolomite	0.01	-17.08	-17.09	CaMg (CO3) 2
Epsomite	-4.10	-6.24	-2.14	MgSO4:7H2O
Fe (OH) 2 (1)	-5.86	7.08	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-6.81	7.08	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-7.21	-2.32	4.89	Fe (OH) 3

FeO	-6.51	7.08	13.59	FeO
FeS (pom)	-0.68	-4.59	-3.91	FeS
FeS (ppt)	-0.67	-4.59	-3.92	FeS
Fluorite	-1.11	-11.71	-10.60	CaF2
Goethite	-1.32	-2.32	-1.00	FeOOH
Greigite	-5.48	-44.25	-38.77	Fe3S4
Gypsum	-1.13	-5.71	-4.58	CaSO4:2H2O
H2 (g)	-7.23	-10.38	-3.15	H2
H2O (g)	-1.51	-0.00	1.51	H2O
H2S (g)	-3.73	-4.73	-1.00	H2S
Halite	-7.72	-6.14	1.58	NaCl
Hausmannite	-29.51	31.52	61.03	Mn3O4
Hematite	-0.64	-4.65	-4.01	Fe2O3
Jarosite-H3O	-27.64	-39.75	-12.11	H3OFe3 (SO4) 2 (OH) 6
Jarosite-K	-25.60	-36.60	-11.00	KFe3 (SO4) 2 (OH) 6
Lepidocrocite	-6.00	10.70	16.70	FeOOH
Lime	-12.13	10.68	22.81	Ca (OH) 2
Mackinawite	0.05	-4.59	-4.64	FeS
Mackinawite(2)	-1.15	2.35	3.50	FeS
Magnetite	-17.32	28.48	45.80	Fe3O4
Manganite	-13.63	11.71	25.34	MnOOH
Marcasite	8.74	-9.03	-17.76	FeS2
Melanterite	-7.10	-9.31	-2.21	FeSO4:7H2O
Nesquehonite	-3.18	-8.80	-5.62	MgCO3:3H2O
O2 (g)	-68.66	-71.62	-2.96	O2
Pyrite	9.45	-9.03	-18.48	FeS2
Pyrochroite	-7.10	8.10	15.20	Mn (OH) 2
Pyrolusite	-26.05	15.33	41.38	MnO2
Rhodochrosite	0.27	-10.86	-11.13	MnCO3
Schwertmannite(1)	-58.59	-48.09	10.50	Fe8O8 (OH) 4.4 (SO4) 1.8:8.4H2O
Schwertmannite(2)	-52.97	-34.97	18.00	Fe8O8 (OH) 6SO4
Siderite	-0.99	-11.88	-10.89	FeCO3
Sulfur	-2.38	2.50	4.88	S
Troilite	1.57	-4.59	-6.16	FeS

End of simulation.

Reading input data for simulation 7.

SOLUTION 1 MWT-22 1-10-08 (downgradient of Biowall B2)

temp	25
pH	6.68
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
Cl	47
F	0.25
S(6)	100 as SO4
S(-2)	1.6 as S

N(5) 1.0
 N(3) 1.5
 Ca 310
 Fe 3.5
 Mg 52
 Mn 5.7
 K 8.3
 Na 110
 Alkalinity 490 as HCO3
 water 1 # kg

END

 Beginning of initial solution calculations.

Initial solution 1. MWT-22 1-10-08 (downgradient of Biowall B2)

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	8.030e-003	8.030e-003
Ca	7.735e-003	7.735e-003
Cl	1.326e-003	1.326e-003
F	1.316e-005	1.316e-005
Fe	6.267e-005	6.267e-005
K	2.123e-004	2.123e-004
Mg	2.139e-003	2.139e-003
Mn	1.038e-004	1.038e-004
N(3)	1.071e-004	1.071e-004
N(5)	7.139e-005	7.139e-005
Na	4.785e-003	4.785e-003
S(-2)	4.990e-005	4.990e-005
S(6)	1.041e-003	1.041e-003

-----Description of solution-----

pH	=	6.680
pe	=	4.000
Activity of water	=	1.000
Ionic strength	=	2.682e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	1.097e-002
Total CO2 (mol/kg)	=	1.097e-002
Temperature (deg C)	=	25.000
Electrical balance (eq)	=	1.345e-002
Percent error, 100*(Cat- An)/(Cat+ An)	=	39.50
Iterations	=	9
Total H	=	1.110205e+002
Total O	=	5.554073e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
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N (3) /N (5)	7.5171	0.4447
S (-2) /S (6)	-3.1259	-0.1849

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.378e-007	2.089e-007	-6.624	-6.680	-0.056
OH-	5.629e-008	4.789e-008	-7.250	-7.320	-0.070
H2O	5.551e+001	9.995e-001	1.744	-0.000	0.000
C (4)	1.097e-002				
HCO3-	7.436e-003	6.408e-003	-2.129	-2.193	-0.065
CO2	2.993e-003	3.012e-003	-2.524	-2.521	0.003
CaHCO3+	3.702e-004	3.190e-004	-3.432	-3.496	-0.065
MgHCO3+	9.558e-005	8.181e-005	-4.020	-4.087	-0.068
MnHCO3+	2.625e-005	2.247e-005	-4.581	-4.648	-0.068
FeHCO3+	1.491e-005	1.276e-005	-4.826	-4.894	-0.068
NaHCO3	1.463e-005	1.472e-005	-4.835	-4.832	0.003
CaCO3	9.371e-006	9.429e-006	-5.028	-5.026	0.003
MnCO3	4.467e-006	4.495e-006	-5.350	-5.347	0.003
CO3-2	2.609e-006	1.438e-006	-5.584	-5.842	-0.259
MgCO3	1.488e-006	1.498e-006	-5.827	-5.825	0.003
FeCO3	6.830e-007	6.872e-007	-6.166	-6.163	0.003
NaCO3-	1.278e-007	1.094e-007	-6.893	-6.961	-0.068
Fe (CO3) (OH) -	1.494e-008	1.279e-008	-7.826	-7.893	-0.068
Fe (CO3) 2-2	2.164e-009	1.161e-009	-8.665	-8.935	-0.270
Ca	7.735e-003				
Ca+2	7.077e-003	3.902e-003	-2.150	-2.409	-0.259
CaHCO3+	3.702e-004	3.190e-004	-3.432	-3.496	-0.065
CaSO4	2.777e-004	2.794e-004	-3.556	-3.554	0.003
CaCO3	9.371e-006	9.429e-006	-5.028	-5.026	0.003
CaF+	4.012e-007	3.434e-007	-6.397	-6.464	-0.068
CaOH+	3.620e-009	3.098e-009	-8.441	-8.509	-0.068
CaHSO4+	3.996e-010	3.420e-010	-9.398	-9.466	-0.068
Cl	1.326e-003				
Cl-	1.325e-003	1.129e-003	-2.878	-2.947	-0.070
MnCl+	2.113e-007	1.809e-007	-6.675	-6.743	-0.068
FeCl+	3.625e-008	3.103e-008	-7.441	-7.508	-0.068
MnCl2	8.857e-011	8.912e-011	-10.053	-10.050	0.003
MnCl3-	3.237e-014	2.770e-014	-13.490	-13.557	-0.068
FeCl+2	9.040e-023	4.852e-023	-22.044	-22.314	-0.270
FeCl2+	2.858e-025	2.446e-025	-24.544	-24.612	-0.068
FeCl3	2.744e-029	2.761e-029	-28.562	-28.559	0.003
F	1.316e-005				
F-	1.187e-005	1.010e-005	-4.925	-4.996	-0.070
MgF+	8.508e-007	7.283e-007	-6.070	-6.138	-0.068
CaF+	4.012e-007	3.434e-007	-6.397	-6.464	-0.068
NaF	2.360e-008	2.374e-008	-7.627	-7.624	0.003
MnF+	3.212e-009	2.750e-009	-8.493	-8.561	-0.068
HF	3.146e-009	3.165e-009	-8.502	-8.500	0.003
FeF+	2.351e-009	2.012e-009	-8.629	-8.696	-0.068
HF2-	1.434e-013	1.227e-013	-12.844	-12.911	-0.068

FeF+2	4.246e-020	2.279e-020	-19.372	-19.642	-0.270
FeF2+	1.071e-020	9.166e-021	-19.970	-20.038	-0.068
FeF3	1.459e-022	1.468e-022	-21.836	-21.833	0.003
Fe (2)	6.267e-005				
Fe+2	3.560e-005	1.992e-005	-4.449	-4.701	-0.252
FeHCO3+	1.491e-005	1.276e-005	-4.826	-4.894	-0.068
FeS	7.407e-006	7.453e-006	-5.130	-5.128	0.003
Fe (HS) 2	2.709e-006	2.726e-006	-5.567	-5.565	0.003
FeSO4	1.263e-006	1.271e-006	-5.898	-5.896	0.003
FeCO3	6.830e-007	6.872e-007	-6.166	-6.163	0.003
FeCl+	3.625e-008	3.103e-008	-7.441	-7.508	-0.068
FeOH+	3.520e-008	3.013e-008	-7.453	-7.521	-0.068
Fe (CO3) (OH) -	1.494e-008	1.279e-008	-7.826	-7.893	-0.068
Fe (HS) 3-	4.297e-009	3.678e-009	-8.367	-8.434	-0.068
FeF+	2.351e-009	2.012e-009	-8.629	-8.696	-0.068
Fe (CO3) 2-2	2.164e-009	1.161e-009	-8.665	-8.935	-0.270
FeHSO4+	2.040e-012	1.746e-012	-11.690	-11.758	-0.068
Fe (OH) 2	1.112e-012	1.119e-012	-11.954	-11.951	0.003
Fe (3)	1.243e-013				
Fe (OH) 2+	8.137e-014	6.965e-014	-13.090	-13.157	-0.068
Fe (OH) 3	4.266e-014	4.292e-014	-13.370	-13.367	0.003
Fe (OH) 4-	2.188e-016	1.873e-016	-15.660	-15.728	-0.068
FeOH+2	8.192e-017	4.396e-017	-16.087	-16.357	-0.270
FeF+2	4.246e-020	2.279e-020	-19.372	-19.642	-0.270
FeF2+	1.071e-020	9.166e-021	-19.970	-20.038	-0.068
FeSO4+	6.544e-021	5.601e-021	-20.184	-20.252	-0.068
Fe+3	4.562e-021	1.423e-021	-20.341	-20.847	-0.506
FeF3	1.459e-022	1.468e-022	-21.836	-21.833	0.003
FeCl+2	9.040e-023	4.852e-023	-22.044	-22.314	-0.270
Fe (SO4) 2-	5.138e-023	4.398e-023	-22.289	-22.357	-0.068
FeCl2+	2.858e-025	2.446e-025	-24.544	-24.612	-0.068
FeHSO4+2	5.839e-027	3.134e-027	-26.234	-26.504	-0.270
FeCl3	2.744e-029	2.761e-029	-28.562	-28.559	0.003
Fe2 (OH) 2+4	6.271e-031	5.202e-032	-30.203	-31.284	-1.081
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-40.432	-42.121	-1.689
H (0)	1.097e-010				
H2	5.485e-011	5.519e-011	-10.261	-10.258	0.003
K	2.123e-004				
K+	2.117e-004	1.803e-004	-3.674	-3.744	-0.070
KSO4-	5.312e-007	4.547e-007	-6.275	-6.342	-0.068
KOH	2.972e-012	2.991e-012	-11.527	-11.524	0.003
Mg	2.139e-003				
Mg+2	1.950e-003	1.091e-003	-2.710	-2.962	-0.252
MgHCO3+	9.558e-005	8.181e-005	-4.020	-4.087	-0.068
MgSO4	9.123e-005	9.180e-005	-4.040	-4.037	0.003
MgCO3	1.488e-006	1.498e-006	-5.827	-5.825	0.003
MgF+	8.508e-007	7.283e-007	-6.070	-6.138	-0.068
MgOH+	9.555e-009	8.178e-009	-8.020	-8.087	-0.068
Mn (2)	1.038e-004				
Mn+2	7.032e-005	3.934e-005	-4.153	-4.405	-0.252
MnHCO3+	2.625e-005	2.247e-005	-4.581	-4.648	-0.068
MnCO3	4.467e-006	4.495e-006	-5.350	-5.347	0.003
MnSO4	2.495e-006	2.511e-006	-5.603	-5.600	0.003
MnCl+	2.113e-007	1.809e-007	-6.675	-6.743	-0.068

MnOH+	5.652e-009	4.838e-009	-8.248	-8.315	-0.068
MnF+	3.212e-009	2.750e-009	-8.493	-8.561	-0.068
MnCl2	8.857e-011	8.912e-011	-10.053	-10.050	0.003
Mn (NO3) 2	5.700e-013	5.735e-013	-12.244	-12.241	0.003
MnCl3-	3.237e-014	2.770e-014	-13.490	-13.557	-0.068
Mn (3)	3.690e-033				
Mn+3	3.690e-033	9.097e-034	-32.433	-33.041	-0.608
N (3)	1.071e-004				
NO2-	1.071e-004	9.077e-005	-3.970	-4.042	-0.072
N (5)	7.139e-005				
NO3-	7.139e-005	6.051e-005	-4.146	-4.218	-0.072
Mn (NO3) 2	5.700e-013	5.735e-013	-12.244	-12.241	0.003
Na	4.785e-003				
Na+	4.761e-003	4.084e-003	-2.322	-2.389	-0.067
NaHCO3	1.463e-005	1.472e-005	-4.835	-4.832	0.003
NaSO4-	8.583e-006	7.346e-006	-5.066	-5.134	-0.068
NaCO3-	1.278e-007	1.094e-007	-6.893	-6.961	-0.068
NaF	2.360e-008	2.374e-008	-7.627	-7.624	0.003
NaOH	1.283e-010	1.291e-010	-9.892	-9.889	0.003
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-71.867	-71.864	0.003
S (-2)	4.990e-005				
H2S	2.250e-005	2.264e-005	-4.648	-4.645	0.003
HS-	1.457e-005	1.239e-005	-4.837	-4.907	-0.070
FeS	7.407e-006	7.453e-006	-5.130	-5.128	0.003
Fe (HS) 2	2.709e-006	2.726e-006	-5.567	-5.565	0.003
Fe (HS) 3-	4.297e-009	3.678e-009	-8.367	-8.434	-0.068
S-2	1.312e-011	7.163e-012	-10.882	-11.145	-0.263
S (6)	1.041e-003				
SO4-2	6.591e-004	3.589e-004	-3.181	-3.445	-0.264
CaSO4	2.777e-004	2.794e-004	-3.556	-3.554	0.003
MgSO4	9.123e-005	9.180e-005	-4.040	-4.037	0.003
NaSO4-	8.583e-006	7.346e-006	-5.066	-5.134	-0.068
MnSO4	2.495e-006	2.511e-006	-5.603	-5.600	0.003
FeSO4	1.263e-006	1.271e-006	-5.898	-5.896	0.003
KSO4-	5.312e-007	4.547e-007	-6.275	-6.342	-0.068
HSO4-	8.518e-009	7.290e-009	-8.070	-8.137	-0.068
CaHSO4+	3.996e-010	3.420e-010	-9.398	-9.466	-0.068
FeHSO4+	2.040e-012	1.746e-012	-11.690	-11.758	-0.068
FeSO4+	6.544e-021	5.601e-021	-20.184	-20.252	-0.068
Fe (SO4) 2-	5.138e-023	4.398e-023	-22.289	-22.357	-0.068
FeHSO4+2	5.839e-027	3.134e-027	-26.234	-26.504	-0.270

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-2.22	20.87	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	4.54	29.53	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-9.04	33.08	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-18.49	39.86	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-18.12	42.26	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-15.00	28.56	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-1.49	-5.85	-4.36	CaSO4

Aragonite	0.09	-8.25	-8.34	CaCO3
Brucite	-6.39	10.40	16.79	Mg (OH) 2
Calcite	0.23	-8.25	-8.48	CaCO3
CO2 (g)	-1.05	-2.52	-1.47	CO2
Dolomite	0.03	-17.06	-17.09	CaMg (CO3) 2
Epsomite	-4.27	-6.41	-2.14	MgSO4:7H2O
Fe (OH) 2 (1)	-4.28	8.66	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-5.23	8.66	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-5.70	-0.81	4.89	Fe (OH) 3
FeO	-4.93	8.66	13.59	FeO
FeS (pom)	0.98	-2.93	-3.91	FeS
FeS (ppt)	0.99	-2.93	-3.92	FeS
Fluorite	-1.80	-12.40	-10.60	CaF2
Goethite	0.19	-0.81	-1.00	FeOOH
Greigite	-0.53	-39.30	-38.77	Fe3S4
Gypsum	-1.27	-5.85	-4.58	CaSO4:2H2O
H2 (g)	-7.11	-10.26	-3.15	H2
H2O (g)	-1.51	-0.00	1.51	H2O
H2S (g)	-3.65	-4.65	-1.00	H2S
Halite	-6.92	-5.34	1.58	NaCl
Hausmannite	-27.06	33.97	61.03	Mn3O4
Hematite	2.39	-1.61	-4.01	Fe2O3
Jarosite-H3O	-23.92	-36.03	-12.11	H3OFe3 (SO4) 2 (OH) 6
Jarosite-K	-22.10	-33.10	-11.00	KFe3 (SO4) 2 (OH) 6
Lepidocrocite	-4.49	12.21	16.70	FeOOH
Lime	-11.86	10.95	22.81	Ca (OH) 2
Mackinawite	1.71	-2.93	-4.64	FeS
Mackinawite(2)	0.51	4.01	3.50	FeS
Magnetite	-12.71	33.09	45.80	Fe3O4
Manganite	-12.83	12.51	25.34	MnOOH
Marcasite	10.36	-7.41	-17.76	FeS2
Melanterite	-5.94	-8.15	-2.21	FeSO4:7H2O
Nesquehonite	-3.18	-8.80	-5.62	MgCO3:3H2O
O2 (g)	-68.90	-71.86	-2.96	O2
Pyrite	11.07	-7.41	-18.48	FeS2
Pyrochroite	-6.25	8.95	15.20	Mn (OH) 2
Pyrolusite	-25.32	16.06	41.38	MnO2
Rhodochrosite	0.88	-10.25	-11.13	MnCO3
Schwertmannite(1)	-47.21	-36.71	10.50	Fe8O8 (OH) 4.4 (SO4) 1.8:8.4H2O
Schwertmannite(2)	-41.26	-23.26	18.00	Fe8O8 (OH) 6SO4
Siderite	0.35	-10.54	-10.89	FeCO3
Sulfur	-2.42	2.46	4.88	S
Troilite	3.23	-2.93	-6.16	FeS

End of simulation.

Reading input data for simulation 8.

SOLUTION 1 PT-22 1-10-08 (Between Biowalls B and C)
temp 25

pH 7.44
 pe 4
 redox S(-2)/S(6)
 units mg/kgw
 density 1
 Cl 130
 F 0.8
 S(6) 170 as SO4
 S(-2) 1.6 as S
 N(5) 0.99
 N(3) 0.25
 Ca 130
 Fe 0.3
 Mg 36
 Mn 0.097
 K 9.2
 Na 29
 Alkalinity 1320 as HCO3
 water 1 # kg

END

 Beginning of initial solution calculations.

Initial solution 1. PT-22 1-10-08 (Between Biowalls B and C)

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	2.163e-002	2.163e-002
Ca	3.244e-003	3.244e-003
Cl	3.667e-003	3.667e-003
F	4.211e-005	4.211e-005
Fe	5.372e-006	5.372e-006
K	2.353e-004	2.353e-004
Mg	1.481e-003	1.481e-003
Mn	1.766e-006	1.766e-006
N(3)	1.785e-005	1.785e-005
N(5)	7.068e-005	7.068e-005
Na	1.261e-003	1.261e-003
S(-2)	4.990e-005	4.990e-005
S(6)	1.770e-003	1.770e-003

-----Description of solution-----

pH	=	7.440
pe	=	4.000
Activity of water	=	0.999
Ionic strength	=	2.373e-002
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	2.294e-002
Total CO2 (mol/kg)	=	2.294e-002
Temperature (deg C)	=	25.000

Electrical balance (eq) = -1.801e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -48.59
Iterations = 8
Total H = 1.110339e+002
Total O = 5.558090e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
N(3)/N(5)	7.1440	0.4226
S(-2)/S(6)	-3.9883	-0.2359

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
OH-	3.213e-007	2.756e-007	-6.493	-6.560	-0.067
H+	4.111e-008	3.631e-008	-7.386	-7.440	-0.054
H2O	5.551e+001	9.994e-001	1.744	-0.000	0.000
C(4)	2.294e-002				
HCO3-	2.080e-002	1.805e-002	-1.682	-1.744	-0.062
CO2	1.466e-003	1.474e-003	-2.834	-2.832	0.002
CaHCO3+	3.867e-004	3.355e-004	-3.413	-3.474	-0.062
MgHCO3+	1.652e-004	1.424e-004	-3.782	-3.846	-0.064
CaCO3	5.675e-005	5.706e-005	-4.246	-4.244	0.002
CO3-2	4.112e-005	2.331e-005	-4.386	-4.632	-0.247
MgCO3	1.492e-005	1.500e-005	-4.826	-4.824	0.002
NaHCO3	1.086e-005	1.092e-005	-4.964	-4.962	0.002
FeHCO3+	1.029e-006	8.873e-007	-5.988	-6.052	-0.064
MnHCO3+	5.877e-007	5.068e-007	-6.231	-6.295	-0.064
MnCO3	5.802e-007	5.834e-007	-6.236	-6.234	0.002
NaCO3-	5.415e-007	4.669e-007	-6.266	-6.331	-0.064
FeCO3	2.734e-007	2.749e-007	-6.563	-6.561	0.002
Fe(CO3)(OH)-	3.415e-008	2.944e-008	-7.467	-7.531	-0.064
Fe(CO3)2-2	1.362e-008	7.529e-009	-7.866	-8.123	-0.257
Ca	3.244e-003				
Ca+2	2.571e-003	1.457e-003	-2.590	-2.836	-0.247
CaHCO3+	3.867e-004	3.355e-004	-3.413	-3.474	-0.062
CaSO4	2.286e-004	2.298e-004	-3.641	-3.639	0.002
CaCO3	5.675e-005	5.706e-005	-4.246	-4.244	0.002
CaF+	5.027e-007	4.335e-007	-6.299	-6.363	-0.064
CaOH+	7.720e-009	6.657e-009	-8.112	-8.177	-0.064
CaHSO4+	5.670e-011	4.889e-011	-10.246	-10.311	-0.064
Cl	3.667e-003				
Cl-	3.667e-003	3.148e-003	-2.436	-2.502	-0.066
MnCl+	4.686e-009	4.041e-009	-8.329	-8.394	-0.064
FeCl+	2.478e-009	2.136e-009	-8.606	-8.670	-0.064
MnCl2	5.522e-012	5.552e-012	-11.258	-11.256	0.002
MnCl3-	5.582e-015	4.813e-015	-14.253	-14.318	-0.064
FeCl+2	8.295e-025	4.585e-025	-24.081	-24.339	-0.257
FeCl2+	7.477e-027	6.447e-027	-26.126	-26.191	-0.064
FeCl3	2.018e-030	2.029e-030	-29.695	-29.693	0.002

F	4.211e-005					
F-	3.982e-005	3.415e-005	-4.400	-4.467	-0.067	
MgF+	1.765e-006	1.522e-006	-5.753	-5.818	-0.064	
CaF+	5.027e-007	4.335e-007	-6.299	-6.363	-0.064	
NaF	2.103e-008	2.114e-008	-7.677	-7.675	0.002	
HF	1.850e-009	1.860e-009	-8.733	-8.731	0.002	
FeF+	1.948e-010	1.679e-010	-9.711	-9.775	-0.064	
MnF+	8.634e-011	7.445e-011	-10.064	-10.128	-0.064	
HF2-	2.826e-013	2.437e-013	-12.549	-12.613	-0.064	
FeF+2	4.723e-022	2.611e-022	-21.326	-21.583	-0.257	
FeF2+	4.117e-022	3.550e-022	-21.385	-21.450	-0.064	
FeF3	1.911e-023	1.921e-023	-22.719	-22.716	0.002	
Fe (2)	5.372e-006					
FeS	2.660e-006	2.675e-006	-5.575	-5.573	0.002	
FeHCO3+	1.029e-006	8.873e-007	-5.988	-6.052	-0.064	
Fe+2	8.560e-007	4.917e-007	-6.068	-6.308	-0.241	
Fe (HS) 2	4.271e-007	4.294e-007	-6.369	-6.367	0.002	
FeCO3	2.734e-007	2.749e-007	-6.563	-6.561	0.002	
FeSO4	6.874e-008	6.912e-008	-7.163	-7.160	0.002	
Fe (CO3) (OH) -	3.415e-008	2.944e-008	-7.467	-7.531	-0.064	
Fe (CO3) 2-2	1.362e-008	7.529e-009	-7.866	-8.123	-0.257	
FeOH+	4.964e-009	4.280e-009	-8.304	-8.369	-0.064	
FeCl+	2.478e-009	2.136e-009	-8.606	-8.670	-0.064	
Fe (HS) 3-	1.698e-009	1.464e-009	-8.770	-8.834	-0.064	
FeF+	1.948e-010	1.679e-010	-9.711	-9.775	-0.064	
Fe (OH) 2	9.096e-013	9.146e-013	-12.041	-12.039	0.002	
FeHSO4+	1.913e-014	1.650e-014	-13.718	-13.783	-0.064	
Fe (3)	3.743e-014					
Fe (OH) 3	2.756e-014	2.771e-014	-13.560	-13.557	0.002	
Fe (OH) 2+	9.062e-015	7.814e-015	-14.043	-14.107	-0.064	
Fe (OH) 4-	8.067e-016	6.956e-016	-15.093	-15.158	-0.064	
FeOH+2	1.551e-018	8.573e-019	-17.809	-18.067	-0.257	
FeF+2	4.723e-022	2.611e-022	-21.326	-21.583	-0.257	
FeF2+	4.117e-022	3.550e-022	-21.385	-21.450	-0.064	
FeSO4+	4.849e-023	4.181e-023	-22.314	-22.379	-0.064	
FeF3	1.911e-023	1.921e-023	-22.719	-22.716	0.002	
Fe+3	1.474e-023	4.824e-024	-22.831	-23.317	-0.485	
Fe (SO4) 2-	8.385e-025	7.230e-025	-24.076	-24.141	-0.064	
FeCl+2	8.295e-025	4.585e-025	-24.081	-24.339	-0.257	
FeCl2+	7.477e-027	6.447e-027	-26.126	-26.191	-0.064	
FeHSO4+2	7.353e-030	4.065e-030	-29.134	-29.391	-0.257	
FeCl3	2.018e-030	2.029e-030	-29.695	-29.693	0.002	
Fe2 (OH) 2+4	2.118e-034	1.978e-035	-33.674	-34.704	-1.030	
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-44.882	-46.491	-1.609	
H (0)	1.759e-010					
H2	8.796e-011	8.845e-011	-10.056	-10.053	0.002	
K	2.353e-004					
K+	2.340e-004	2.009e-004	-3.631	-3.697	-0.066	
KSO4-	1.294e-006	1.116e-006	-5.888	-5.952	-0.064	
KOH	1.907e-011	1.917e-011	-10.720	-10.717	0.002	
Mg	1.481e-003					
Mg+2	1.174e-003	6.746e-004	-2.930	-3.171	-0.241	
MgHCO3+	1.652e-004	1.424e-004	-3.782	-3.846	-0.064	
MgSO4	1.243e-004	1.250e-004	-3.905	-3.903	0.002	

MgCO ₃	1.492e-005	1.500e-005	-4.826	-4.824	0.002
MgF ⁺	1.765e-006	1.522e-006	-5.753	-5.818	-0.064
MgOH ⁺	3.374e-008	2.909e-008	-7.472	-7.536	-0.064
Mn (2)	1.766e-006				
MnHCO ₃ ⁺	5.877e-007	5.068e-007	-6.231	-6.295	-0.064
MnCO ₃	5.802e-007	5.834e-007	-6.236	-6.234	0.002
Mn ⁺²	5.486e-007	3.151e-007	-6.261	-6.502	-0.241
MnSO ₄	4.405e-008	4.429e-008	-7.356	-7.354	0.002
MnCl ⁺	4.686e-009	4.041e-009	-8.329	-8.394	-0.064
MnOH ⁺	2.586e-010	2.230e-010	-9.587	-9.652	-0.064
MnF ⁺	8.634e-011	7.445e-011	-10.064	-10.128	-0.064
MnCl ₂	5.522e-012	5.552e-012	-11.258	-11.256	0.002
MnCl ₃ ⁻	5.582e-015	4.813e-015	-14.253	-14.318	-0.064
Mn (NO ₃) ₂	4.554e-015	4.579e-015	-14.342	-14.339	0.002
Mn (3)	3.796e-036				
Mn ⁺³	3.796e-036	1.000e-036	-35.421	-36.000	-0.579
N (3)	1.785e-005				
NO ₂ ⁻	1.785e-005	1.526e-005	-4.748	-4.817	-0.068
N (5)	7.068e-005				
NO ₃ ⁻	7.068e-005	6.042e-005	-4.151	-4.219	-0.068
Mn (NO ₃) ₂	4.554e-015	4.579e-015	-14.342	-14.339	0.002
Na	1.261e-003				
Na ⁺	1.245e-003	1.076e-003	-2.905	-2.968	-0.063
NaHCO ₃	1.086e-005	1.092e-005	-4.964	-4.962	0.002
NaSO ₄ ⁻	4.943e-006	4.262e-006	-5.306	-5.370	-0.064
NaCO ₃ ⁻	5.415e-007	4.669e-007	-6.266	-6.331	-0.064
NaF	2.103e-008	2.114e-008	-7.677	-7.675	0.002
NaOH	1.946e-010	1.956e-010	-9.711	-9.709	0.002
O (0)	0.000e+000				
O ₂	0.000e+000	0.000e+000	-72.276	-72.274	0.002
S (-2)	4.990e-005				
HS ⁻	3.650e-005	3.130e-005	-4.438	-4.504	-0.067
H ₂ S	9.883e-006	9.937e-006	-5.005	-5.003	0.002
FeS	2.660e-006	2.675e-006	-5.575	-5.573	0.002
Fe (HS) ₂	4.271e-007	4.294e-007	-6.369	-6.367	0.002
Fe (HS) ₃ ⁻	1.698e-009	1.464e-009	-8.770	-8.834	-0.064
S ⁻²	1.854e-010	1.041e-010	-9.732	-9.982	-0.250
S (6)	1.770e-003				
SO ₄ ⁻²	1.410e-003	7.905e-004	-2.851	-3.102	-0.251
CaSO ₄	2.286e-004	2.298e-004	-3.641	-3.639	0.002
MgSO ₄	1.243e-004	1.250e-004	-3.905	-3.903	0.002
NaSO ₄ ⁻	4.943e-006	4.262e-006	-5.306	-5.370	-0.064
KSO ₄ ⁻	1.294e-006	1.116e-006	-5.888	-5.952	-0.064
FeSO ₄	6.874e-008	6.912e-008	-7.163	-7.160	0.002
MnSO ₄	4.405e-008	4.429e-008	-7.356	-7.354	0.002
HSO ₄ ⁻	3.236e-009	2.790e-009	-8.490	-8.554	-0.064
CaHSO ₄ ⁺	5.670e-011	4.889e-011	-10.246	-10.311	-0.064
FeHSO ₄ ⁺	1.913e-014	1.650e-014	-13.718	-13.783	-0.064
FeSO ₄ ⁺	4.849e-023	4.181e-023	-22.314	-22.379	-0.064
Fe (SO ₄) ₂ ⁻	8.385e-025	7.230e-025	-24.076	-24.141	-0.064
FeHSO ₄ ⁺²	7.353e-030	4.065e-030	-29.134	-29.391	-0.257

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH)5]	-2.50	20.59	23.09	Fe2(OH)5
[Fe3(OH)7]	4.18	29.17	24.99	Fe3(OH)7
[Fe3(OH)8]	-9.50	32.62	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-19.53	38.82	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-20.03	40.35	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-15.77	27.79	43.56	Fe4(OH)8(Cl)1
Anhydrite	-1.58	-5.94	-4.36	CaSO4
Aragonite	0.87	-7.47	-8.34	CaCO3
Brucite	-5.08	11.71	16.79	Mg(OH)2
Calcite	1.01	-7.47	-8.48	CaCO3
CO2(g)	-1.36	-2.83	-1.47	CO2
Dolomite	1.82	-15.27	-17.09	CaMg(CO3)2
Epsomite	-4.13	-6.27	-2.14	MgSO4·7H2O
Fe(OH)2(1)	-4.37	8.57	12.94	Fe(OH)2
Fe(OH)2(2)	-5.32	8.57	13.89	Fe(OH)2
Fe(OH)3(a)	-5.89	-1.00	4.89	Fe(OH)3
FeO	-5.02	8.57	13.59	FeO
FeS(pom)	0.54	-3.37	-3.91	FeS
FeS(ppt)	0.54	-3.37	-3.92	FeS
Fluorite	-1.17	-11.77	-10.60	CaF2
Goethite	0.00	-1.00	-1.00	FeOOH
Greigite	-2.43	-41.20	-38.77	Fe3S4
Gypsum	-1.36	-5.94	-4.58	CaSO4·2H2O
H2(g)	-6.90	-10.05	-3.15	H2
H2O(g)	-1.51	-0.00	1.51	H2O
H2S(g)	-4.01	-5.00	-1.00	H2S
Halite	-7.05	-5.47	1.58	NaCl
Hausmannite	-28.99	32.04	61.03	Mn3O4
Hematite	2.01	-1.99	-4.01	Fe2O3
Jarosite-H3O	-26.85	-38.96	-12.11	H3OFe3(SO4)2(OH)6
Jarosite-K	-24.21	-35.21	-11.00	KFe3(SO4)2(OH)6
Lepidocrocite	-4.68	12.02	16.70	FeOOH
Lime	-10.77	12.04	22.81	Ca(OH)2
Mackinawite	1.27	-3.37	-4.64	FeS
Mackinawite(2)	0.07	3.57	3.50	FeS
Magnetite	-13.18	32.62	45.80	Fe3O4
Manganite	-13.51	11.83	25.34	MnOOH
Marcasite	9.35	-8.41	-17.76	FeS2
Melanterite	-7.20	-9.41	-2.21	FeSO4·7H2O
Nesquehonite	-2.18	-7.80	-5.62	MgCO3·3H2O
O2(g)	-69.31	-72.27	-2.96	O2
Pyrite	10.07	-8.41	-18.48	FeS2
Pyrochroite	-6.82	8.38	15.20	Mn(OH)2
Pyrolusite	-26.10	15.28	41.38	MnO2
Rhodochrosite	-0.00	-11.13	-11.13	MnCO3
Schwertmannite(1)	-50.85	-40.35	10.50	Fe8O8(OH)4.4(SO4)1.8·8.4H2O
Schwertmannite(2)	-43.96	-25.96	18.00	Fe8O8(OH)6SO4
Siderite	-0.05	-10.94	-10.89	FeCO3
Sulfur	-2.98	1.90	4.88	S
Troilite	2.79	-3.37	-6.16	FeS

End of simulation.

Reading input data for simulation 9.

End of run.

Dugway PG

Input file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\Dugway.pqi
Output file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\Dugway.pqi
Database file: C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\phreeqc8.dat

Reading data base.

SOLUTION_MASTER_SPECIES
SOLUTION_SPECIES
PHASES
EXCHANGE_MASTER_SPECIES
EXCHANGE_SPECIES
SURFACE_MASTER_SPECIES
SURFACE_SPECIES
RATES
END

Reading input data for simulation 1.

DATABASE C:\Documents and Settings\whitingks\My Documents\Program
Files\USGS\Phreeqc Interactive 2.6\phreeqc8.dat

SOLUTION 1 Dugway TW-22 (Downgradient) 4-24-2008

temp	13.8
pH	6.20
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
S(-2)	0.656
S(6)	11600 as SO4
Ca	850
K	550
Mg	2000
Na	15000
Alkalinity	611 as CaCO3
Fe	6.47
Mn	1.5
Cl	27100
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 1. Dugway TW-22 (Downgradient) 4-24-2008

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455
g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	1.221e-002	1.221e-002
Ca	2.121e-002	2.121e-002
Cl	7.644e-001	7.644e-001
Fe	1.159e-004	1.159e-004
K	1.407e-002	1.407e-002
Mg	8.226e-002	8.226e-002
Mn	2.730e-005	2.730e-005
Na	6.525e-001	6.525e-001
S (-2)	2.046e-005	2.046e-005
S (6)	1.208e-001	1.208e-001

-----Description of solution-----

pH = 6.200
 pe = 4.000
 Activity of water = 0.973
 Ionic strength = 9.916e-001
 Mass of water (kg) = 1.000e+000
 Total carbon (mol/kg) = 2.053e-002
 Total CO2 (mol/kg) = 2.053e-002
 Temperature (deg C) = 13.800
 Electrical balance (eq) = -1.443e-001
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -8.43
 Iterations = 8
 Total H = 1.110247e+002
 Total O = 5.604249e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2)/S (6)	-2.0970	-0.1194

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	8.450e-007	6.310e-007	-6.073	-6.200	-0.127
OH-	1.073e-008	6.276e-009	-7.969	-8.202	-0.233
H2O	5.551e+001	9.725e-001	1.744	-0.012	0.000
C (4)	2.053e-002				
HCO3-	9.121e-003	6.016e-003	-2.040	-2.221	-0.181
CO2	8.337e-003	1.048e-002	-2.079	-1.980	0.099
MgHCO3+	1.477e-003	1.171e-003	-2.831	-2.931	-0.101
NaHCO3	1.212e-003	1.523e-003	-2.916	-2.817	0.099
CaHCO3+	3.627e-004	2.392e-004	-3.440	-3.621	-0.181
FeHCO3+	1.177e-005	9.334e-006	-4.929	-5.030	-0.101
MgCO3	3.801e-006	4.776e-006	-5.420	-5.321	0.099
NaCO3-	2.025e-006	1.606e-006	-5.693	-5.794	-0.101
MnHCO3+	1.981e-006	1.571e-006	-5.703	-5.804	-0.101

		CO3-2	1.821e-006	3.445e-007	-5.740	-6.463	-0.723
		CaCO3	1.499e-006	1.884e-006	-5.824	-5.725	0.099
		FeCO3	1.021e-007	1.282e-007	-6.991	-6.892	0.099
		MnCO3	6.381e-008	8.018e-008	-7.195	-7.096	0.099
		Fe (CO3) (OH) -	9.698e-010	7.689e-010	-9.013	-9.114	-0.101
		Fe (CO3) 2-2	1.313e-010	5.191e-011	-9.882	-10.285	-0.403
Ca	2.121e-002						
		Ca+2	1.526e-002	3.875e-003	-1.817	-2.412	-0.595
		CaSO4	5.587e-003	7.020e-003	-2.253	-2.154	0.099
		CaHCO3+	3.627e-004	2.392e-004	-3.440	-3.621	-0.181
		CaCO3	1.499e-006	1.884e-006	-5.824	-5.725	0.099
		CaHSO4+	2.891e-008	2.292e-008	-7.539	-7.640	-0.101
		CaOH+	1.250e-009	9.912e-010	-8.903	-9.004	-0.101
Cl	7.644e-001						
		Cl-	7.644e-001	4.626e-001	-0.117	-0.335	-0.218
		FeCl+	1.249e-005	9.907e-006	-4.903	-5.004	-0.101
		MnCl+	6.963e-006	5.521e-006	-5.157	-5.258	-0.101
		MnCl2	8.872e-007	1.115e-006	-6.052	-5.953	0.099
		MnCl3-	1.791e-007	1.420e-007	-6.747	-6.848	-0.101
		FeCl2+	2.280e-019	1.808e-019	-18.642	-18.743	-0.101
		FeCl+2	1.531e-019	6.051e-020	-18.815	-19.218	-0.403
		FeCl3	6.657e-021	8.364e-021	-20.177	-20.078	0.099
Fe (2)	1.159e-004						
		Fe+2	7.344e-005	1.551e-005	-4.134	-4.809	-0.675
		FeSO4	1.797e-005	2.258e-005	-4.746	-4.646	0.099
		FeCl+	1.249e-005	9.907e-006	-4.903	-5.004	-0.101
		FeHCO3+	1.177e-005	9.334e-006	-4.929	-5.030	-0.101
		FeCO3	1.021e-007	1.282e-007	-6.991	-6.892	0.099
		Fe (HS) 2	6.950e-008	8.733e-008	-7.158	-7.059	0.099
		FeOH+	3.998e-009	3.170e-009	-8.398	-8.499	-0.101
		Fe (CO3) (OH) -	9.698e-010	7.689e-010	-9.013	-9.114	-0.101
		Fe (CO3) 2-2	1.313e-010	5.191e-011	-9.882	-10.285	-0.403
		FeHSO4+	1.158e-010	9.179e-011	-9.936	-10.037	-0.101
		Fe (HS) 3-	3.014e-011	2.390e-011	-10.521	-10.622	-0.101
		Fe (OH) 2	7.201e-014	9.048e-014	-13.143	-13.043	0.099
Fe (3)	1.407e-014						
		Fe (OH) 2+	1.301e-014	1.031e-014	-13.886	-13.987	-0.101
		Fe (OH) 3	9.814e-016	1.233e-015	-15.008	-14.909	0.099
		FeOH+2	7.950e-017	3.142e-017	-16.100	-16.503	-0.403
		Fe (OH) 4-	1.370e-018	1.086e-018	-17.863	-17.964	-0.101
		FeSO4+	6.777e-019	5.373e-019	-18.169	-18.270	-0.101
		FeCl2+	2.280e-019	1.808e-019	-18.642	-18.743	-0.101
		FeCl+2	1.531e-019	6.051e-020	-18.815	-19.218	-0.403
		Fe (SO4) 2-	1.434e-019	1.137e-019	-18.843	-18.944	-0.101
		Fe+3	8.681e-020	6.264e-021	-19.061	-20.203	-1.142
		FeCl3	6.657e-021	8.364e-021	-20.177	-20.078	0.099
		FeHSO4+2	2.355e-024	9.308e-025	-23.628	-24.031	-0.403
		Fe2 (OH) 2+4	1.761e-030	4.298e-032	-29.754	-31.367	-1.613
		Fe3 (OH) 4+5	0.000e+000	0.000e+000	-40.047	-42.567	-2.520
H (0)	7.874e-012						
		H2	3.937e-012	4.947e-012	-11.405	-11.306	0.099
K	1.407e-002						
		K+	1.347e-002	8.151e-003	-1.871	-2.089	-0.218
		KSO4-	5.968e-004	4.732e-004	-3.224	-3.325	-0.101

KOH	3.467e-011	4.356e-011	-10.460	-10.361	0.099
Mg	8.226e-002				
Mg+2	5.664e-002	1.725e-002	-1.247	-1.763	-0.516
MgSO4	2.415e-002	3.034e-002	-1.617	-1.518	0.099
MgHCO3+	1.477e-003	1.171e-003	-2.831	-2.931	-0.101
MgCO3	3.801e-006	4.776e-006	-5.420	-5.321	0.099
MgOH+	1.837e-008	1.457e-008	-7.736	-7.837	-0.101
Mn (2)	2.730e-005				
Mn+2	1.387e-005	2.930e-006	-4.858	-5.533	-0.675
MnCl+	6.963e-006	5.521e-006	-5.157	-5.258	-0.101
MnSO4	3.362e-006	4.224e-006	-5.473	-5.374	0.099
MnHCO3+	1.981e-006	1.571e-006	-5.703	-5.804	-0.101
MnCl2	8.872e-007	1.115e-006	-6.052	-5.953	0.099
MnCl3-	1.791e-007	1.420e-007	-6.747	-6.848	-0.101
MnCO3	6.381e-008	8.018e-008	-7.195	-7.096	0.099
MnOH+	5.669e-011	4.495e-011	-10.246	-10.347	-0.101
Mn (3)	1.069e-033				
Mn+3	1.069e-033	1.323e-034	-32.971	-33.878	-0.907
Na	6.525e-001				
Na+	6.245e-001	4.502e-001	-0.204	-0.347	-0.142
NaSO4-	2.676e-002	2.121e-002	-1.573	-1.673	-0.101
NaHCO3	1.212e-003	1.523e-003	-2.916	-2.817	0.099
NaCO3-	2.025e-006	1.606e-006	-5.693	-5.794	-0.101
NaOH	3.649e-009	4.584e-009	-8.438	-8.339	0.099
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-73.648	-73.548	0.099
S (-2)	2.046e-005				
H2S	1.602e-005	2.013e-005	-4.795	-4.696	0.099
HS-	4.297e-006	2.513e-006	-5.367	-5.600	-0.233
Fe (HS) 2	6.950e-008	8.733e-008	-7.158	-7.059	0.099
Fe (HS) 3-	3.014e-011	2.390e-011	-10.521	-10.622	-0.101
S-2	1.244e-012	2.168e-013	-11.905	-12.664	-0.759
S (6)	1.208e-001				
SO4-2	6.365e-002	1.012e-002	-1.196	-1.995	-0.798
NaSO4-	2.676e-002	2.121e-002	-1.573	-1.673	-0.101
MgSO4	2.415e-002	3.034e-002	-1.617	-1.518	0.099
CaSO4	5.587e-003	7.020e-003	-2.253	-2.154	0.099
KSO4-	5.968e-004	4.732e-004	-3.224	-3.325	-0.101
FeSO4	1.797e-005	2.258e-005	-4.746	-4.646	0.099
MnSO4	3.362e-006	4.224e-006	-5.473	-5.374	0.099
HSO4-	6.206e-007	4.921e-007	-6.207	-6.308	-0.101
CaHSO4+	2.891e-008	2.292e-008	-7.539	-7.640	-0.101
FeHSO4+	1.158e-010	9.179e-011	-9.936	-10.037	-0.101
FeSO4+	6.777e-019	5.373e-019	-18.169	-18.270	-0.101
Fe (SO4) 2-	1.434e-019	1.137e-019	-18.843	-18.944	-0.101
FeHSO4+2	2.355e-024	9.308e-025	-23.628	-24.031	-0.403

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-3.87	19.22	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	1.80	26.79	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-11.24	30.88	42.12	Fe3 (OH) 8

[Fe6(OH)12][CO3]	-23.61	34.74	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-21.17	39.21	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-15.73	27.83	43.56	Fe4(OH)8(Cl)1
Anhydrite	-0.07	-4.41	-4.33	CaSO4
Aragonite	-0.60	-8.87	-8.27	CaCO3
Brucite	-6.18	10.61	16.79	Mg(OH)2
Calcite	-0.45	-8.87	-8.43	CaCO3
CO2(g)	-0.66	-1.98	-1.32	CO2
Dolomite	-0.28	-17.10	-16.82	CaMg(CO3)2
Epsomite	-1.62	-3.84	-2.22	MgSO4:7H2O
Fe(OH)2(1)	-5.37	7.57	12.94	Fe(OH)2
Fe(OH)2(2)	-6.32	7.57	13.89	Fe(OH)2
Fe(OH)3(a)	-6.53	-1.64	4.89	Fe(OH)3
FeO	-6.01	7.58	13.59	FeO
FeS(am)	-0.43	-4.21	-3.78	FeS
FeS(ppt)	-0.29	-4.21	-3.92	FeS
Goethite	-1.04	-1.63	-0.59	FeOOH
Greigite	-4.30	-42.81	-38.51	Fe3S4
Gypsum	0.16	-4.43	-4.59	CaSO4:2H2O
H2(g)	-8.21	-11.31	-3.10	H2
H2O(g)	-1.82	-0.01	1.81	H2O
H2S(g)	-3.83	-4.70	-0.87	H2S
Halite	-2.24	-0.68	1.56	NaCl
Hausmannite	-35.15	28.76	63.91	Mn3O4
Hematite	-0.12	-3.24	-3.13	Fe2O3
Jarosite-H3O	-23.15	-33.68	-10.53	H3OFe3(SO4)2(OH)6
Jarosite-K	-18.87	-29.56	-10.69	KFe3(SO4)2(OH)6
Lepidocrocite	-5.03	11.67	16.70	FeOOH
Lime	-12.85	9.96	22.81	Ca(OH)2
Mackinawite	0.33	-4.21	-4.54	FeS
Magnetite	-14.87	30.93	45.80	Fe3O4
Manganite	-14.39	10.95	25.34	MnOOH
Marcasite	10.26	-7.80	-18.06	FeS2
Melanterite	-4.53	-6.89	-2.36	FeSO4:7H2O
Nesquehonite	-2.81	-8.26	-5.46	MgCO3:3H2O
O2(g)	-70.64	-73.55	-2.91	O2
Pyrite	11.00	-7.80	-18.80	FeS2
Pyrochroite	-8.36	6.84	15.20	Mn(OH)2
Pyrolusite	-28.19	15.05	43.24	MnO2
Rhodochrosite	-0.91	-12.00	-11.09	MnCO3
Schwertmannite(1)	-49.49	-38.99	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-45.39	-27.39	18.00	Fe8O8(OH)6SO4
Siderite	-0.45	-11.27	-10.82	FeCO3
Sulfur	-1.64	3.51	5.15	S
Troilite	1.92	-4.21	-6.13	FeS

End of simulation.

Reading input data for simulation 2.

SOLUTION 2 Dugway TW-23 (Downgradient) 4-24-2008

temp 13.5
pH 5.69
pe 4
redox S(-2)/S(6)
units mg/kgw
density 1
S(-2) 0.3
S(6) 11200 as SO4
Ca 860
K 690
Mg 2300
Na 16000
Alkalinity 1286 as CaCO3
Fe 11.0
Mn 1.6
Cl 29600
water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 2. Dugway TW-23 (Downgradient) 4-24-2008

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	2.570e-002	2.570e-002
Ca	2.146e-002	2.146e-002
Cl	8.349e-001	8.349e-001
Fe	1.970e-004	1.970e-004
K	1.765e-002	1.765e-002
Mg	9.460e-002	9.460e-002
Mn	2.912e-005	2.912e-005
Na	6.960e-001	6.960e-001
S(-2)	9.356e-006	9.356e-006
S(6)	1.166e-001	1.166e-001

-----Description of solution-----

pH	=	5.690
pe	=	4.000
Activity of water	=	0.969
Ionic strength	=	1.067e+000
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	8.044e-002
Total CO2 (mol/kg)	=	8.044e-002
Temperature (deg C)	=	13.500
Electrical balance (eq)	=	-1.476e-001
Percent error, 100*(Cat- An)/(Cat+ An)	=	-7.97

Iterations = 10
 Total H = 1.110381e+002
 Total O = 5.615914e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2) / S (6)	-1.4246	-0.0810

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	2.742e-006	2.042e-006	-5.562	-5.690	-0.128
OH-	3.252e-009	1.885e-009	-8.488	-8.725	-0.237
H2O	5.551e+001	9.694e-001	1.744	-0.013	0.000
C (4)	8.044e-002				
CO2	5.474e-002	6.999e-002	-1.262	-1.155	0.107
HCO3-	1.876e-002	1.231e-002	-1.727	-1.910	-0.183
MgHCO3+	3.505e-003	2.823e-003	-2.455	-2.549	-0.094
NaHCO3	2.619e-003	3.349e-003	-2.582	-2.475	0.107
CaHCO3+	7.600e-004	4.986e-004	-3.119	-3.302	-0.183
FeHCO3+	3.651e-005	2.940e-005	-4.438	-4.532	-0.094
MnHCO3+	3.895e-006	3.137e-006	-5.410	-5.504	-0.094
MgCO3	2.749e-006	3.514e-006	-5.561	-5.454	0.107
NaCO3-	1.322e-006	1.065e-006	-5.879	-5.973	-0.094
CO3-2	1.167e-006	2.161e-007	-5.933	-6.665	-0.732
CaCO3	9.456e-007	1.209e-006	-6.024	-5.918	0.107
FeCO3	9.685e-008	1.238e-007	-7.014	-6.907	0.107
MnCO3	3.839e-008	4.908e-008	-7.416	-7.309	0.107
Fe (CO3) (OH) -	2.840e-010	2.287e-010	-9.547	-9.641	-0.094
Fe (CO3) 2-2	7.473e-011	3.144e-011	-10.127	-10.503	-0.376
Ca	2.146e-002				
Ca+2	1.558e-002	3.977e-003	-1.807	-2.400	-0.593
CaSO4	5.117e-003	6.543e-003	-2.291	-2.184	0.107
CaHCO3+	7.600e-004	4.986e-004	-3.119	-3.302	-0.183
CaCO3	9.456e-007	1.209e-006	-6.024	-5.918	0.107
CaHSO4+	8.560e-008	6.894e-008	-7.068	-7.162	-0.094
CaOH+	3.891e-010	3.134e-010	-9.410	-9.504	-0.094
Cl	8.349e-001				
Cl-	8.349e-001	5.020e-001	-0.078	-0.299	-0.221
FeCl+	2.055e-005	1.655e-005	-4.687	-4.781	-0.094
MnCl+	7.261e-006	5.848e-006	-5.139	-5.233	-0.094
MnCl2	1.002e-006	1.282e-006	-5.999	-5.892	0.107
MnCl3-	2.200e-007	1.772e-007	-6.658	-6.752	-0.094
FeCl2+	1.881e-018	1.515e-018	-17.726	-17.820	-0.094
FeCl+2	1.099e-018	4.623e-019	-17.959	-18.335	-0.376
FeCl3	5.948e-020	7.605e-020	-19.226	-19.119	0.107
Fe (2)	1.970e-004				
Fe+2	1.152e-004	2.388e-005	-3.939	-4.622	-0.683
FeHCO3+	3.651e-005	2.940e-005	-4.438	-4.532	-0.094
FeSO4	2.462e-005	3.147e-005	-4.609	-4.502	0.107

FeCl+	2.055e-005	1.655e-005	-4.687	-4.781	-0.094
FeCO3	9.685e-008	1.238e-007	-7.014	-6.907	0.107
Fe (HS) 2	2.946e-009	3.767e-009	-8.531	-8.424	0.107
FeOH+	1.822e-009	1.467e-009	-8.740	-8.834	-0.094
FeHSO4+	5.141e-010	4.141e-010	-9.289	-9.383	-0.094
Fe (CO3) (OH) -	2.840e-010	2.287e-010	-9.547	-9.641	-0.094
Fe (CO3) 2-2	7.473e-011	3.144e-011	-10.127	-10.503	-0.376
Fe (HS) 3-	2.143e-013	1.726e-013	-12.669	-12.763	-0.094
Fe (OH) 2	1.034e-014	1.322e-014	-13.986	-13.879	0.107
Fe (3)	8.738e-015				
Fe (OH) 2+	8.377e-015	6.746e-015	-14.077	-14.171	-0.094
Fe (OH) 3	1.916e-016	2.450e-016	-15.718	-15.611	0.107
FeOH+2	1.605e-016	6.754e-017	-15.794	-16.170	-0.376
FeSO4+	4.292e-018	3.457e-018	-17.367	-17.461	-0.094
FeCl2+	1.881e-018	1.515e-018	-17.726	-17.820	-0.094
FeCl+2	1.099e-018	4.623e-019	-17.959	-18.335	-0.376
Fe (SO4) 2-	8.263e-019	6.655e-019	-18.083	-18.177	-0.094
Fe+3	6.321e-019	4.455e-020	-18.199	-19.351	-1.152
Fe (OH) 4-	8.145e-020	6.560e-020	-19.089	-19.183	-0.094
FeCl3	5.948e-020	7.605e-020	-19.226	-19.119	0.107
FeHSO4+2	4.611e-023	1.940e-023	-22.336	-22.712	-0.376
Fe2 (OH) 2+4	6.424e-030	2.013e-031	-29.192	-30.696	-1.504
Fe3 (OH) 4+5	1.915e-040	0.000e+000	-39.718	-42.068	-2.350
H (0)	3.675e-012				
H2	1.837e-012	2.349e-012	-11.736	-11.629	0.107
K	1.765e-002				
K+	1.698e-002	1.021e-002	-1.770	-1.991	-0.221
KSO4-	6.667e-004	5.369e-004	-3.176	-3.270	-0.094
KOH	1.315e-011	1.681e-011	-10.881	-10.774	0.107
Mg	9.460e-002				
Mg+2	6.583e-002	2.033e-002	-1.182	-1.692	-0.510
MgSO4	2.526e-002	3.230e-002	-1.598	-1.491	0.107
MgHCO3+	3.505e-003	2.823e-003	-2.455	-2.549	-0.094
MgCO3	2.749e-006	3.514e-006	-5.561	-5.454	0.107
MgOH+	6.377e-009	5.136e-009	-8.195	-8.289	-0.094
Mn (2)	2.912e-005				
Mn+2	1.379e-005	2.859e-006	-4.860	-5.544	-0.683
MnCl+	7.261e-006	5.848e-006	-5.139	-5.233	-0.094
MnHCO3+	3.895e-006	3.137e-006	-5.410	-5.504	-0.094
MnSO4	2.919e-006	3.732e-006	-5.535	-5.428	0.107
MnCl2	1.002e-006	1.282e-006	-5.999	-5.892	0.107
MnCl3-	2.200e-007	1.772e-007	-6.658	-6.752	-0.094
MnCO3	3.839e-008	4.908e-008	-7.416	-7.309	0.107
MnOH+	1.634e-011	1.316e-011	-10.787	-10.881	-0.094
Mn (3)	4.064e-033				
Mn+3	4.064e-033	5.794e-034	-32.391	-33.237	-0.846
Na	6.960e-001				
Na+	6.676e-001	4.838e-001	-0.175	-0.315	-0.140
NaSO4-	2.573e-002	2.073e-002	-1.589	-1.683	-0.094
NaHCO3	2.619e-003	3.349e-003	-2.582	-2.475	0.107
NaCO3-	1.322e-006	1.065e-006	-5.879	-5.973	-0.094
NaOH	1.187e-009	1.518e-009	-8.926	-8.819	0.107
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-73.116	-73.009	0.107

S (-2)	9.356e-006					
H2S	8.625e-006	1.103e-005	-5.064	-4.958	0.107	
HS-	7.258e-007	4.207e-007	-6.139	-6.376	-0.237	
Fe (HS) 2	2.946e-009	3.767e-009	-8.531	-8.424	0.107	
Fe (HS) 3-	2.143e-013	1.726e-013	-12.669	-12.763	-0.094	
S-2	6.445e-014	1.097e-014	-13.191	-13.960	-0.769	
S (6)	1.166e-001					
SO4-2	5.978e-002	9.221e-003	-1.223	-2.035	-0.812	
NaSO4-	2.573e-002	2.073e-002	-1.589	-1.683	-0.094	
MgSO4	2.526e-002	3.230e-002	-1.598	-1.491	0.107	
CaSO4	5.117e-003	6.543e-003	-2.291	-2.184	0.107	
KSO4-	6.667e-004	5.369e-004	-3.176	-3.270	-0.094	
FeSO4	2.462e-005	3.147e-005	-4.609	-4.502	0.107	
MnSO4	2.919e-006	3.732e-006	-5.535	-5.428	0.107	
HSO4-	1.790e-006	1.442e-006	-5.747	-5.841	-0.094	
CaHSO4+	8.560e-008	6.894e-008	-7.068	-7.162	-0.094	
FeHSO4+	5.141e-010	4.141e-010	-9.289	-9.383	-0.094	
FeSO4+	4.292e-018	3.457e-018	-17.367	-17.461	-0.094	
Fe (SO4) 2-	8.263e-019	6.655e-019	-18.083	-18.177	-0.094	
FeHSO4+2	4.611e-023	1.940e-023	-22.336	-22.712	-0.376	

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2 (OH) 5]	-5.38	17.71	23.09	Fe2 (OH) 5
[Fe3 (OH) 7]	-0.54	24.45	24.99	Fe3 (OH) 7
[Fe3 (OH) 8]	-13.42	28.70	42.12	Fe3 (OH) 8
[Fe6 (OH) 12] [CO3]	-27.48	30.87	58.35	Fe6 (OH) 12 (CO3) 1
[Fe6 (OH) 12] [SO4]	-24.88	35.50	60.38	Fe6 (OH) 12 (SO4) 1
[Fe6 (OH) 8] [Cl]	-18.36	25.20	43.56	Fe4 (OH) 8 (Cl) 1
Anhydrite	-0.10	-4.44	-4.33	CaSO4
Aragonite	-0.79	-9.07	-8.27	CaCO3
Brucite	-7.13	9.66	16.79	Mg (OH) 2
Calcite	-0.64	-9.07	-8.42	CaCO3
CO2 (g)	0.17	-1.15	-1.32	CO2
Dolomite	-0.61	-17.42	-16.81	CaMg (CO3) 2
Epsomite	-1.60	-3.82	-2.22	MgSO4:7H2O
Fe (OH) 2 (1)	-6.21	6.73	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-7.16	6.73	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-7.21	-2.32	4.89	Fe (OH) 3
FeO	-6.85	6.74	13.59	FeO
FeS (am)	-1.53	-5.31	-3.78	FeS
FeS (ppt)	-1.39	-5.31	-3.92	FeS
Goethite	-1.73	-2.31	-0.57	FeOOH
Greigite	-7.56	-46.07	-38.51	Fe3S4
Gypsum	0.12	-4.46	-4.59	CaSO4:2H2O
H2 (g)	-8.53	-11.63	-3.10	H2
H2O (g)	-1.83	-0.01	1.82	H2O
H2S (g)	-4.09	-4.96	-0.86	H2S
Halite	-2.17	-0.61	1.56	NaCl
Hausmannite	-38.00	25.99	63.99	Mn3O4
Hematite	-1.50	-4.60	-3.10	Fe2O3
Jarosite-H3O	-23.28	-33.77	-10.49	H3OFe3 (SO4) 2 (OH) 6

Jarosite-K	-19.37	-30.06	-10.68	KFe3(SO4)2(OH)6
Lepidocrocite	-5.70	11.00	16.70	FeOOH
Lime	-13.86	8.95	22.81	Ca(OH)2
Mackinawite	-0.77	-5.31	-4.54	FeS
Magnetite	-17.05	28.75	45.80	Fe3O4
Manganite	-15.27	10.07	25.34	MnOOH
Marcasite	9.22	-8.84	-18.07	FeS2
Melanterite	-4.39	-6.75	-2.36	FeSO4·7H2O
Nesquehonite	-2.95	-8.40	-5.45	MgCO3·3H2O
O2(g)	-70.10	-73.01	-2.91	O2
Pyrite	9.97	-8.84	-18.81	FeS2
Pyrochroite	-9.39	5.81	15.20	Mn(OH)2
Pyrolusite	-28.95	14.34	43.29	MnO2
Rhodochrosite	-1.12	-12.21	-11.09	MnCO3
Schwertmannite(1)	-53.18	-42.68	10.50	Fe8O8(OH)4.4(SO4)1.8·8.4H2O
Schwertmannite(2)	-49.85	-31.85	18.00	Fe8O8(OH)6SO4
Siderite	-0.47	-11.29	-10.82	FeCO3
Sulfur	-1.59	3.57	5.16	S
Troilite	0.82	-5.31	-6.13	FeS

End of simulation.

Reading input data for simulation 3.

SOLUTION 3 Dugway TW-24 (Downgradient) 4-22-2008

temp	14.9
pH	5.38
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
S(-2)	0.003
S(6)	11600 as SO4
Ca	770
K	660
Mg	2000
Na	18000
Alkalinity	249 as CaCO3
Fe	0.035
Mn	0.034
Cl	29800
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 3. Dugway TW-24 (Downgradient) 4-22-2008

WARNING: Equivalent wt for alkalinity should be $\text{Ca} \cdot 5(\text{CO}_3) \cdot 5$. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	4.975e-003	4.975e-003
Ca	1.921e-002	1.921e-002
Cl	8.405e-001	8.405e-001
Fe	6.267e-007	6.267e-007
K	1.688e-002	1.688e-002
Mg	8.226e-002	8.226e-002
Mn	6.189e-007	6.189e-007
Na	7.830e-001	7.830e-001
S (-2)	9.356e-008	9.356e-008
S (6)	1.208e-001	1.208e-001

-----Description of solution-----

pH	=	5.380
pe	=	4.000
Activity of water	=	0.969
Ionic strength	=	1.090e+000
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	2.610e-002
Total CO2 (mol/kg)	=	2.610e-002
Temperature (deg C)	=	14.900
Electrical balance (eq)	=	-8.424e-002
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	-4.40
Iterations	=	11
Total H	=	1.110174e+002
Total O	=	5.604641e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S (-2) / S (6)	-0.8188	-0.0468

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	5.605e-006	4.169e-006	-5.251	-5.380	-0.129
OH-	1.799e-009	1.039e-009	-8.745	-8.983	-0.238
H2O	5.551e+001	9.689e-001	1.744	-0.014	0.000
C (4)	2.610e-002				
CO2	2.111e-002	2.714e-002	-1.675	-1.566	0.109
HCO3-	3.667e-003	2.400e-003	-2.436	-2.620	-0.184
MgHCO3+	6.029e-004	4.877e-004	-3.220	-3.312	-0.092
NaHCO3	5.732e-004	7.368e-004	-3.242	-3.133	0.109
CaHCO3+	1.403e-004	9.185e-005	-3.853	-4.037	-0.184
MgCO3	2.446e-007	3.144e-007	-6.612	-6.503	0.109

	NaCO3-	1.588e-007	1.285e-007	-6.799	-6.891	-0.092
	CO3-2	1.167e-007	2.142e-008	-6.933	-7.669	-0.736
	CaCO3	8.645e-008	1.111e-007	-7.063	-6.954	0.109
	FeHCO3+	2.620e-008	2.120e-008	-7.582	-7.674	-0.092
	MnHCO3+	1.786e-008	1.445e-008	-7.748	-7.840	-0.092
	MnCO3	8.938e-011	1.149e-010	-10.049	-9.940	0.109
	FeCO3	3.529e-011	4.537e-011	-10.452	-10.343	0.109
	Fe (CO3) (OH) -	5.071e-014	4.102e-014	-13.295	-13.387	-0.092
	Fe (CO3) 2-2	2.665e-015	1.141e-015	-14.574	-14.943	-0.368
Ca	1.921e-002					
	Ca+2	1.425e-002	3.633e-003	-1.846	-2.440	-0.594
	CaSO4	4.820e-003	6.196e-003	-2.317	-2.208	0.109
	CaHCO3+	1.403e-004	9.185e-005	-3.853	-4.037	-0.184
	CaHSO4+	1.670e-007	1.351e-007	-6.777	-6.869	-0.092
	CaCO3	8.645e-008	1.111e-007	-7.063	-6.954	0.109
	CaOH+	1.732e-010	1.401e-010	-9.761	-9.853	-0.092
Cl	8.405e-001					
	Cl-	8.405e-001	5.040e-001	-0.075	-0.298	-0.222
	MnCl+	1.714e-007	1.387e-007	-6.766	-6.858	-0.092
	FeCl+	7.594e-008	6.144e-008	-7.120	-7.212	-0.092
	MnCl2	2.373e-008	3.051e-008	-7.625	-7.516	0.109
	MnCl3-	5.235e-009	4.235e-009	-8.281	-8.373	-0.092
	FeCl2+	3.057e-020	2.473e-020	-19.515	-19.607	-0.092
	FeCl+2	1.841e-020	7.887e-021	-19.735	-20.103	-0.368
	FeCl3	9.698e-022	1.247e-021	-21.013	-20.904	0.109
Fe (2)	6.267e-007					
	Fe+2	4.294e-007	8.831e-008	-6.367	-7.054	-0.687
	FeSO4	9.510e-008	1.222e-007	-7.022	-6.913	0.109
	FeCl+	7.594e-008	6.144e-008	-7.120	-7.212	-0.092
	FeHCO3+	2.620e-008	2.120e-008	-7.582	-7.674	-0.092
	FeCO3	3.529e-011	4.537e-011	-10.452	-10.343	0.109
	FeHSO4+	4.060e-012	3.284e-012	-11.392	-11.484	-0.092
	FeOH+	3.674e-012	2.972e-012	-11.435	-11.527	-0.092
	Fe (CO3) (OH) -	5.071e-014	4.102e-014	-13.295	-13.387	-0.092
	Fe (CO3) 2-2	2.665e-015	1.141e-015	-14.574	-14.943	-0.368
	Fe (HS) 2	3.144e-016	4.041e-016	-15.503	-15.394	0.109
	Fe (OH) 2	9.110e-018	1.171e-017	-17.040	-16.931	0.109
	Fe (HS) 3-	1.232e-022	9.970e-023	-21.909	-22.001	-0.092
Fe (3)	3.942e-017					
	Fe (OH) 2+	3.746e-017	3.030e-017	-16.426	-16.519	-0.092
	FeOH+2	1.366e-018	5.853e-019	-17.864	-18.233	-0.368
	Fe (OH) 3	4.475e-019	5.753e-019	-18.349	-18.240	0.109
	FeSO4+	7.315e-020	5.918e-020	-19.136	-19.228	-0.092
	FeCl2+	3.057e-020	2.473e-020	-19.515	-19.607	-0.092
	FeCl+2	1.841e-020	7.887e-021	-19.735	-20.103	-0.368
	Fe (SO4) 2-	1.448e-020	1.171e-020	-19.839	-19.931	-0.092
	Fe+3	1.036e-020	7.218e-022	-19.985	-21.142	-1.157
	FeCl3	9.698e-022	1.247e-021	-21.013	-20.904	0.109
	Fe (OH) 4-	9.902e-023	8.011e-023	-22.004	-22.096	-0.092
	FeHSO4+2	1.574e-024	6.743e-025	-23.803	-24.171	-0.368
	Fe2 (OH) 2+4	4.218e-034	1.420e-035	-33.375	-34.848	-1.473
	Fe3 (OH) 4+5	0.000e+000	0.000e+000	-46.326	-48.627	-2.301
H (0)	9.222e-013					
	H2	4.611e-013	5.927e-013	-12.336	-12.227	0.109

K	1.688e-002					
K+	1.622e-002	9.723e-003	-1.790	-2.012	-0.222	
KSO4-	6.632e-004	5.365e-004	-3.178	-3.270	-0.092	
KOH	6.096e-012	7.836e-012	-11.215	-11.106	0.109	
Mg	8.226e-002					
Mg+2	5.807e-002	1.797e-002	-1.236	-1.746	-0.510	
MgSO4	2.359e-002	3.032e-002	-1.627	-1.518	0.109	
MgHCO3+	6.029e-004	4.877e-004	-3.220	-3.312	-0.092	
MgCO3	2.446e-007	3.144e-007	-6.612	-6.503	0.109	
MgOH+	3.146e-009	2.545e-009	-8.502	-8.594	-0.092	
Mn (2)	6.189e-007					
Mn+2	3.284e-007	6.754e-008	-6.484	-7.170	-0.687	
MnCl+	1.714e-007	1.387e-007	-6.766	-6.858	-0.092	
MnSO4	7.213e-008	9.272e-008	-7.142	-7.033	0.109	
MnCl2	2.373e-008	3.051e-008	-7.625	-7.516	0.109	
MnHCO3+	1.786e-008	1.445e-008	-7.748	-7.840	-0.092	
MnCl3-	5.235e-009	4.235e-009	-8.281	-8.373	-0.092	
MnCO3	8.938e-011	1.149e-010	-10.049	-9.940	0.109	
MnOH+	2.127e-013	1.721e-013	-12.672	-12.764	-0.092	
Mn (3)	4.635e-034					
Mn+3	4.635e-034	6.881e-035	-33.334	-34.162	-0.828	
Na	7.830e-001					
Na+	7.526e-001	5.458e-001	-0.123	-0.263	-0.139	
NaSO4-	2.982e-002	2.413e-002	-1.525	-1.617	-0.092	
NaHCO3	5.732e-004	7.368e-004	-3.242	-3.133	0.109	
NaCO3-	1.588e-007	1.285e-007	-6.799	-6.891	-0.092	
NaOH	6.521e-010	8.382e-010	-9.186	-9.077	0.109	
O (0)	0.000e+000					
O2	0.000e+000	0.000e+000	-71.436	-71.327	0.109	
S (-2)	9.356e-008					
H2S	8.964e-008	1.152e-007	-7.048	-6.938	0.109	
HS-	3.924e-009	2.266e-009	-8.406	-8.645	-0.238	
Fe (HS) 2	3.144e-016	4.041e-016	-15.503	-15.394	0.109	
S-2	1.904e-016	3.208e-017	-15.720	-16.494	-0.773	
Fe (HS) 3-	1.232e-022	9.970e-023	-21.909	-22.001	-0.092	
S (6)	1.208e-001					
SO4-2	6.185e-002	9.424e-003	-1.209	-2.026	-0.817	
NaSO4-	2.982e-002	2.413e-002	-1.525	-1.617	-0.092	
MgSO4	2.359e-002	3.032e-002	-1.627	-1.518	0.109	
CaSO4	4.820e-003	6.196e-003	-2.317	-2.208	0.109	
KSO4-	6.632e-004	5.365e-004	-3.178	-3.270	-0.092	
HSO4-	3.824e-006	3.093e-006	-5.418	-5.510	-0.092	
CaHSO4+	1.670e-007	1.351e-007	-6.777	-6.869	-0.092	
FeSO4	9.510e-008	1.222e-007	-7.022	-6.913	0.109	
MnSO4	7.213e-008	9.272e-008	-7.142	-7.033	0.109	
FeHSO4+	4.060e-012	3.284e-012	-11.392	-11.484	-0.092	
FeSO4+	7.315e-020	5.918e-020	-19.136	-19.228	-0.092	
Fe (SO4) 2-	1.448e-020	1.171e-020	-19.839	-19.931	-0.092	
FeHSO4+2	1.574e-024	6.743e-025	-23.803	-24.171	-0.368	

-----Saturation indices-----

Phase

SI log IAP log KT

[Fe2(OH)5]	-11.19	11.90	23.09	Fe2(OH)5
[Fe3(OH)7]	-9.41	15.58	24.99	Fe3(OH)7
[Fe3(OH)8]	-21.99	20.13	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-45.59	12.76	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-41.97	18.41	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-29.96	13.60	43.56	Fe4(OH)8(Cl)1
Anhydrite	-0.13	-4.47	-4.34	CaSO4
Aragonite	-1.83	-10.11	-8.28	CaCO3
Brucite	-7.80	8.99	16.79	Mg(OH)2
Calcite	-1.68	-10.11	-8.43	CaCO3
CO2(g)	-0.23	-1.57	-1.34	CO2
Dolomite	-2.68	-19.52	-16.85	CaMg(CO3)2
Epsomite	-1.65	-3.87	-2.21	MgSO4:7H2O
Fe(OH)2(1)	-9.26	3.68	12.94	Fe(OH)2
Fe(OH)2(2)	-10.21	3.68	13.89	Fe(OH)2
Fe(OH)3(a)	-9.93	-5.04	4.89	Fe(OH)3
FeO	-9.90	3.69	13.59	FeO
FeS(am)	-6.53	-10.32	-3.79	FeS
FeS(ppt)	-6.40	-10.32	-3.92	FeS
Goethite	-4.40	-5.03	-0.63	FeOOH
Greigite	-23.86	-62.40	-38.54	Fe3S4
Gypsum	0.09	-4.49	-4.58	CaSO4:2H2O
H2(g)	-9.12	-12.23	-3.10	H2
H2O(g)	-1.79	-0.01	1.78	H2O
H2S(g)	-6.06	-6.94	-0.88	H2S
Halite	-2.12	-0.56	1.56	NaCl
Hausmannite	-43.78	19.84	63.62	Mn3O4
Hematite	-6.83	-10.04	-3.22	Fe2O3
Jarosite-H3O	-29.98	-40.67	-10.69	H3OFe3(SO4)2(OH)6
Jarosite-K	-26.57	-37.29	-10.72	KFe3(SO4)2(OH)6
Lepidocrocite	-8.46	8.24	16.70	FeOOH
Lime	-14.52	8.29	22.81	Ca(OH)2
Mackinawite	-5.77	-10.32	-4.55	FeS
Magnetite	-25.61	20.19	45.80	Fe3O4
Manganite	-17.22	8.12	25.34	MnOOH
Marcasite	2.81	-15.22	-18.03	FeS2
Melanterite	-6.84	-9.18	-2.34	FeSO4:7H2O
Nesquehonite	-3.98	-9.46	-5.47	MgCO3:3H2O
O2(g)	-68.41	-71.33	-2.91	O2
Pyrite	3.55	-15.22	-18.77	FeS2
Pyrochroite	-11.64	3.56	15.20	Mn(OH)2
Pyrolusite	-30.37	12.68	43.05	MnO2
Rhodochrosite	-3.75	-14.84	-11.09	MnCO3
Schwertmannite(1)	-73.81	-63.31	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-70.99	-52.99	18.00	Fe8O8(OH)6SO4
Siderite	-3.90	-14.72	-10.83	FeCO3
Sulfur	-2.94	2.18	5.13	S
Troilite	-4.19	-10.32	-6.13	FeS

End of simulation.

Reading input data for simulation 4.

SOLUTION 4 Dugway TW-25 (Upgradient) 4-22-2008

temp 14.78
pH 6.23
pe 4
redox S(-2)/S(6)
units mg/kgw
density 1
S(-2) 0.011
S(6) 12400 as SO4
Ca 760
K 740
Mg 2200
Na 17000
Alkalinity 309 as CaCO3
Fe 0.088
Mn 0.092
Cl 24700
water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 4. Dugway TW-25 (Upgradient) 4-22-2008

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	6.174e-003	6.174e-003
Ca	1.896e-002	1.896e-002
Cl	6.967e-001	6.967e-001
Fe	1.576e-006	1.576e-006
K	1.892e-002	1.892e-002
Mg	9.049e-002	9.049e-002
Mn	1.675e-006	1.675e-006
Na	7.395e-001	7.395e-001
S(-2)	3.431e-007	3.431e-007
S(6)	1.291e-001	1.291e-001

-----Description of solution-----

pH	=	6.230
pe	=	4.000
Activity of water	=	0.972
Ionic strength	=	1.012e+000
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	9.931e-003
Total CO2 (mol/kg)	=	9.931e-003

Temperature (deg C) = 14.780
 Electrical balance (eq) = 1.626e-002
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 0.93
 Iterations = 9
 Total H = 1.110186e+002
 Total O = 5.604857e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-1.9326	-0.1104

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	7.895e-007	5.888e-007	-6.103	-6.230	-0.127
OH-	1.253e-008	7.305e-009	-7.902	-8.136	-0.234
H2O	5.551e+001	9.722e-001	1.744	-0.012	0.000
C(4)	9.931e-003				
HCO3-	4.520e-003	2.975e-003	-2.345	-2.526	-0.182
CO2	3.760e-003	4.747e-003	-2.425	-2.324	0.101
MgHCO3+	8.026e-004	6.387e-004	-3.096	-3.195	-0.099
NaHCO3	6.770e-004	8.546e-004	-3.169	-3.068	0.101
CaHCO3+	1.651e-004	1.087e-004	-3.782	-3.964	-0.182
MgCO3	2.298e-006	2.901e-006	-5.639	-5.537	0.101
NaCO3-	1.313e-006	1.045e-006	-5.882	-5.981	-0.099
CO3-2	9.980e-007	1.873e-007	-6.001	-6.727	-0.726
CaCO3	7.361e-007	9.292e-007	-6.133	-6.032	0.101
FeHCO3+	8.342e-008	6.639e-008	-7.079	-7.178	-0.099
MnHCO3+	6.386e-008	5.082e-008	-7.195	-7.294	-0.099
MnCO3	2.259e-009	2.852e-009	-8.646	-8.545	0.101
FeCO3	7.944e-010	1.003e-009	-9.100	-8.999	0.101
Fe(CO3)(OH)-	8.093e-012	6.441e-012	-11.092	-11.191	-0.099
Fe(CO3)2-2	5.502e-013	2.207e-013	-12.259	-12.656	-0.397
Ca	1.896e-002				
Ca+2	1.371e-002	3.477e-003	-1.863	-2.459	-0.596
CaSO4	5.090e-003	6.426e-003	-2.293	-2.192	0.101
CaHCO3+	1.651e-004	1.087e-004	-3.782	-3.964	-0.182
CaCO3	7.361e-007	9.292e-007	-6.133	-6.032	0.101
CaHSO4+	2.484e-008	1.977e-008	-7.605	-7.704	-0.099
CaOH+	1.197e-009	9.527e-010	-8.922	-9.021	-0.099
Cl	6.967e-001				
Cl-	6.967e-001	4.206e-001	-0.157	-0.376	-0.219
MnCl+	4.126e-007	3.284e-007	-6.384	-6.484	-0.099
FeCl+	1.628e-007	1.295e-007	-6.788	-6.888	-0.099
MnCl2	4.776e-008	6.029e-008	-7.321	-7.220	0.101
MnCl3-	8.775e-009	6.984e-009	-8.057	-8.156	-0.099
FeCl2+	4.178e-021	3.325e-021	-20.379	-20.478	-0.099
FeCl+2	3.154e-021	1.266e-021	-20.501	-20.898	-0.397
FeCl3	1.108e-022	1.399e-022	-21.956	-21.854	0.101
Fe(2)	1.576e-006				

Fe+2	1.064e-006	2.231e-007	-5.973	-6.651	-0.678
FeSO4	2.648e-007	3.343e-007	-6.577	-6.476	0.101
FeCl+	1.628e-007	1.295e-007	-6.788	-6.888	-0.099
FeHCO3+	8.342e-008	6.639e-008	-7.079	-7.178	-0.099
FeCO3	7.944e-010	1.003e-009	-9.100	-8.999	0.101
FeOH+	6.638e-011	5.283e-011	-10.178	-10.277	-0.099
Fe (CO3) (OH) -	8.093e-012	6.441e-012	-11.092	-11.191	-0.099
FeHSO4+	1.594e-012	1.269e-012	-11.797	-11.897	-0.099
Fe (CO3) 2-2	5.502e-013	2.207e-013	-12.259	-12.656	-0.397
Fe (HS) 2	3.358e-013	4.239e-013	-12.474	-12.373	0.101
Fe (OH) 2	1.183e-015	1.493e-015	-14.927	-14.826	0.101
Fe (HS) 3-	2.678e-018	2.131e-018	-17.572	-17.671	-0.099
Fe (3)	3.993e-016				
Fe (OH) 2+	3.663e-016	2.915e-016	-15.436	-15.535	-0.099
Fe (OH) 3	3.097e-017	3.909e-017	-16.509	-16.408	0.101
FeOH+2	1.986e-018	7.966e-019	-17.702	-18.099	-0.397
Fe (OH) 4-	4.834e-020	3.847e-020	-19.316	-19.415	-0.099
FeSO4+	1.553e-020	1.236e-020	-19.809	-19.908	-0.099
FeCl2+	4.178e-021	3.325e-021	-20.379	-20.478	-0.099
Fe (SO4) 2-	3.333e-021	2.653e-021	-20.477	-20.576	-0.099
FeCl+2	3.154e-021	1.266e-021	-20.501	-20.898	-0.397
Fe+3	1.950e-021	1.394e-022	-20.710	-21.856	-1.146
FeCl3	1.108e-022	1.399e-022	-21.956	-21.854	0.101
FeHSO4+2	4.961e-026	1.990e-026	-25.304	-25.701	-0.397
Fe2 (OH) 2+4	1.021e-033	2.645e-035	-32.991	-34.578	-1.587
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-44.890	-47.369	-2.479
H (0)	3.169e-012				
H2	1.584e-012	2.000e-012	-11.800	-11.699	0.101
K	1.892e-002				
K+	1.810e-002	1.093e-002	-1.742	-1.961	-0.219
KSO4-	8.202e-004	6.528e-004	-3.086	-3.185	-0.099
KOH	4.956e-011	6.257e-011	-10.305	-10.204	0.101
Mg	9.049e-002				
Mg+2	6.224e-002	1.899e-002	-1.206	-1.722	-0.516
MgSO4	2.745e-002	3.465e-002	-1.562	-1.460	0.101
MgHCO3+	8.026e-004	6.387e-004	-3.096	-3.195	-0.099
MgCO3	2.298e-006	2.901e-006	-5.639	-5.537	0.101
MgOH+	2.373e-008	1.889e-008	-7.625	-7.724	-0.099
Mn (2)	1.675e-006				
Mn+2	9.137e-007	1.917e-007	-6.039	-6.717	-0.678
MnCl+	4.126e-007	3.284e-007	-6.384	-6.484	-0.099
MnSO4	2.256e-007	2.848e-007	-6.647	-6.546	0.101
MnHCO3+	6.386e-008	5.082e-008	-7.195	-7.294	-0.099
MnCl2	4.776e-008	6.029e-008	-7.321	-7.220	0.101
MnCl3-	8.775e-009	6.984e-009	-8.057	-8.156	-0.099
MnCO3	2.259e-009	2.852e-009	-8.646	-8.545	0.101
MnOH+	4.313e-012	3.433e-012	-11.365	-11.464	-0.099
Mn (3)	1.151e-034				
Mn+3	1.151e-034	1.475e-035	-33.939	-34.831	-0.892
Na	7.395e-001				
Na+	7.080e-001	5.107e-001	-0.150	-0.292	-0.142
NaSO4-	3.075e-002	2.447e-002	-1.512	-1.611	-0.099
NaHCO3	6.770e-004	8.546e-004	-3.169	-3.068	0.101
NaCO3-	1.313e-006	1.045e-006	-5.882	-5.981	-0.099

NaOH	4.413e-009	5.571e-009	-8.355	-8.254	0.101
O(0)	0.000e+000				
O2	0.000e+000	0.000e+000	-72.523	-72.422	0.101
S(-2)	3.431e-007				
H2S	2.639e-007	3.331e-007	-6.579	-6.477	0.101
HS-	7.920e-008	4.617e-008	-7.101	-7.336	-0.234
Fe(HS)2	3.358e-013	4.239e-013	-12.474	-12.373	0.101
S-2	2.656e-014	4.587e-015	-13.576	-14.338	-0.763
Fe(HS)3-	2.678e-018	2.131e-018	-17.572	-17.671	-0.099
S(6)	1.291e-001				
SO4-2	6.497e-002	1.022e-002	-1.187	-1.990	-0.803
NaSO4-	3.075e-002	2.447e-002	-1.512	-1.611	-0.099
MgSO4	2.745e-002	3.465e-002	-1.562	-1.460	0.101
CaSO4	5.090e-003	6.426e-003	-2.293	-2.192	0.101
KSO4-	8.202e-004	6.528e-004	-3.086	-3.185	-0.099
HSO4-	5.942e-007	4.729e-007	-6.226	-6.325	-0.099
FeSO4	2.648e-007	3.343e-007	-6.577	-6.476	0.101
MnSO4	2.256e-007	2.848e-007	-6.647	-6.546	0.101
CaHSO4+	2.484e-008	1.977e-008	-7.605	-7.704	-0.099
FeHSO4+	1.594e-012	1.269e-012	-11.797	-11.897	-0.099
FeSO4+	1.553e-020	1.236e-020	-19.809	-19.908	-0.099
Fe(SO4)2-	3.333e-021	2.653e-021	-20.477	-20.576	-0.099
FeHSO4+2	4.961e-026	1.990e-026	-25.304	-25.701	-0.397

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH)5]	-7.24	15.85	23.09	Fe2(OH)5
[Fe3(OH)7]	-3.35	21.64	24.99	Fe3(OH)7
[Fe3(OH)8]	-16.20	25.92	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-34.24	24.11	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-31.53	28.85	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-22.73	20.83	43.56	Fe4(OH)8(Cl)1
Anhydrite	-0.11	-4.45	-4.34	CaSO4
Aragonite	-0.91	-9.19	-8.28	CaCO3
Brucite	-6.08	10.71	16.79	Mg(OH)2
Calcite	-0.76	-9.19	-8.43	CaCO3
CO2(g)	-0.99	-2.32	-1.34	CO2
Dolomite	-0.79	-17.64	-16.84	CaMg(CO3)2
Epsomite	-1.58	-3.80	-2.21	MgSO4:7H2O
Fe(OH)2(1)	-7.16	5.78	12.94	Fe(OH)2
Fe(OH)2(2)	-8.11	5.78	13.89	Fe(OH)2
Fe(OH)3(a)	-8.09	-3.20	4.89	Fe(OH)3
FeO	-7.79	5.80	13.59	FeO
FeS(am)	-3.96	-7.76	-3.79	FeS
FeS(ppt)	-3.84	-7.76	-3.92	FeS
Goethite	-2.57	-3.19	-0.62	FeOOH
Greigite	-16.25	-54.79	-38.54	Fe3S4
Gypsum	0.11	-4.47	-4.58	CaSO4:2H2O
H2(g)	-8.59	-11.70	-3.10	H2
H2O(g)	-1.80	-0.01	1.78	H2O
H2S(g)	-5.60	-6.48	-0.88	H2S
Halite	-2.23	-0.67	1.56	NaCl

Hausmannite	-37.88	25.77	63.65	Mn3O4
Hematite	-3.16	-6.37	-3.21	Fe2O3
Jarosite-H3O	-27.81	-38.48	-10.68	H3OFe3(SO4)2(OH)6
Jarosite-K	-23.48	-34.20	-10.72	KFe3(SO4)2(OH)6
Lepidocrocite	-6.62	10.08	16.70	FeOOH
Lime	-12.83	9.98	22.81	Ca(OH)2
Mackinawite	-3.21	-7.76	-4.55	FeS
Magnetite	-19.83	25.97	45.80	Fe3O4
Manganite	-15.32	10.02	25.34	MnOOH
Marcasite	5.30	-12.73	-18.03	FeS2
Melanterite	-6.39	-8.73	-2.34	FeSO4·7H2O
Nesquehonite	-3.02	-8.49	-5.47	MgCO3·3H2O
O2(g)	-69.51	-72.42	-2.91	O2
Pyrite	6.05	-12.73	-18.77	FeS2
Pyrochroite	-9.48	5.72	15.20	Mn(OH)2
Pyrolusite	-28.76	14.31	43.07	MnO2
Rhodochrosite	-2.35	-13.44	-11.09	MnCO3
Schwertmannite(1)	-62.09	-51.59	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-57.95	-39.95	18.00	Fe8O8(OH)6SO4
Siderite	-2.55	-13.38	-10.83	FeCO3
Sulfur	-3.01	2.12	5.13	S
Troilite	-1.63	-7.76	-6.13	FeS

End of simulation.

Reading input data for simulation 5.

SOLUTION 5 Dugway TW-26 (Crossgradient) 4-22-2008

temp	13.8
pH	6.96
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
S(-2)	0.002
S(6)	11900 as SO4
Ca	760
K	650
Mg	2000
Na	17000
Alkalinity	247 as CaCO3
Fe	0.67
Mn	0.34
Cl	26800
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 5. Dugway TW-26 (Crossgradient) 4-22-2008

WARNING: Equivalent wt for alkalinity should be $\text{Ca} \cdot 5(\text{CO}_3) \cdot 5$. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	4.936e-003	4.936e-003
Ca	1.896e-002	1.896e-002
Cl	7.559e-001	7.559e-001
Fe	1.200e-005	1.200e-005
K	1.662e-002	1.662e-002
Mg	8.226e-002	8.226e-002
Mn	6.189e-006	6.189e-006
Na	7.395e-001	7.395e-001
S(-2)	6.238e-008	6.238e-008
S(6)	1.239e-001	1.239e-001

-----Description of solution-----

pH	=	6.960
pe	=	4.000
Activity of water	=	0.971
Ionic strength	=	1.029e+000
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	5.484e-003
Total CO2 (mol/kg)	=	5.484e-003
Temperature (deg C)	=	13.800
Electrical balance (eq)	=	-5.005e-002
Percent error, $100 \cdot (\text{Cat} - \text{An}) / (\text{Cat} + \text{An})$	=	-2.80
Iterations	=	8
Total H	=	1.110173e+002
Total O	=	5.601760e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.6954	-0.1535

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	1.470e-007	1.096e-007	-6.833	-6.960	-0.127
OH-	6.197e-008	3.608e-008	-7.208	-7.443	-0.235
H2O	5.551e+001	9.714e-001	1.744	-0.013	0.000
C(4)	5.484e-003				
HCO3-	3.626e-003	2.385e-003	-2.441	-2.623	-0.182
MgHCO3+	5.932e-004	4.739e-004	-3.227	-3.324	-0.098
CO2	5.701e-004	7.224e-004	-3.244	-3.141	0.103
NaHCO3	5.422e-004	6.870e-004	-3.266	-3.163	0.103

	CaHCO3+	1.310e-004	8.618e-005	-3.883	-4.065	-0.182
	MgCO3	8.775e-006	1.112e-005	-5.057	-4.954	0.103
	NaCO3-	5.218e-006	4.169e-006	-5.282	-5.380	-0.098
	CO3-2	4.199e-006	7.859e-007	-5.377	-6.105	-0.728
	CaCO3	3.082e-006	3.906e-006	-5.511	-5.408	0.103
	FeHCO3+	5.101e-007	4.075e-007	-6.292	-6.390	-0.098
	MnHCO3+	1.851e-007	1.478e-007	-6.733	-6.830	-0.098
	MnCO3	3.427e-008	4.342e-008	-7.465	-7.362	0.103
	FeCO3	2.542e-008	3.222e-008	-7.595	-7.492	0.103
	Fe (CO3) (OH) -	1.390e-009	1.110e-009	-8.857	-8.955	-0.098
	Fe (CO3) 2-2	7.304e-011	2.975e-011	-10.136	-10.527	-0.390
Ca		1.896e-002				
	Ca+2	1.384e-002	3.522e-003	-1.859	-2.453	-0.594
	CaSO4	4.988e-003	6.321e-003	-2.302	-2.199	0.103
	CaHCO3+	1.310e-004	8.618e-005	-3.883	-4.065	-0.182
	CaCO3	3.082e-006	3.906e-006	-5.511	-5.408	0.103
	CaOH+	6.482e-009	5.178e-009	-8.188	-8.286	-0.098
	CaHSO4+	4.490e-009	3.587e-009	-8.348	-8.445	-0.098
Cl		7.559e-001				
	Cl-	7.559e-001	4.560e-001	-0.122	-0.341	-0.220
	MnCl+	1.617e-006	1.292e-006	-5.791	-5.889	-0.098
	FeCl+	1.346e-006	1.076e-006	-5.871	-5.968	-0.098
	MnCl2	2.029e-007	2.572e-007	-6.693	-6.590	0.103
	MnCl3-	4.043e-008	3.230e-008	-7.393	-7.491	-0.098
	FeCl2+	6.106e-021	4.878e-021	-20.214	-20.312	-0.098
	FeCl+2	4.066e-021	1.656e-021	-20.391	-20.781	-0.390
	FeCl3	1.755e-022	2.224e-022	-21.756	-21.653	0.103
Fe (2)		1.200e-005				
	Fe+2	8.167e-006	1.709e-006	-5.088	-5.767	-0.679
	FeSO4	1.944e-006	2.463e-006	-5.711	-5.608	0.103
	FeCl+	1.346e-006	1.076e-006	-5.871	-5.968	-0.098
	FeHCO3+	5.101e-007	4.075e-007	-6.292	-6.390	-0.098
	FeCO3	2.542e-008	3.222e-008	-7.595	-7.492	0.103
	FeOH+	2.512e-009	2.007e-009	-8.600	-8.698	-0.098
	Fe (CO3) (OH) -	1.390e-009	1.110e-009	-8.857	-8.955	-0.098
	Fe (CO3) 2-2	7.304e-011	2.975e-011	-10.136	-10.527	-0.390
	FeHSO4+	2.179e-012	1.741e-012	-11.662	-11.759	-0.098
	Fe (HS) 2	5.895e-013	7.470e-013	-12.230	-12.127	0.103
	Fe (OH) 2	2.598e-013	3.292e-013	-12.585	-12.482	0.103
	Fe (HS) 3-	2.255e-018	1.801e-018	-17.647	-17.744	-0.098
Fe (3)		1.703e-014				
	Fe (OH) 2+	1.184e-014	9.462e-015	-13.927	-14.024	-0.098
	Fe (OH) 3	5.131e-015	6.503e-015	-14.290	-14.187	0.103
	Fe (OH) 4-	4.120e-017	3.291e-017	-16.385	-16.483	-0.098
	FeOH+2	1.231e-017	5.015e-018	-16.910	-17.300	-0.390
	FeSO4+	1.850e-020	1.478e-020	-19.733	-19.830	-0.098
	FeCl2+	6.106e-021	4.878e-021	-20.214	-20.312	-0.098
	FeCl+2	4.066e-021	1.656e-021	-20.391	-20.781	-0.390
	Fe (SO4) 2-	3.880e-021	3.099e-021	-20.411	-20.509	-0.098
	Fe+3	2.440e-021	1.739e-022	-20.613	-21.760	-1.147
	FeCl3	1.755e-022	2.224e-022	-21.756	-21.653	0.103
	FeHSO4+2	1.093e-026	4.450e-027	-25.962	-26.352	-0.390
	Fe2 (OH) 2+4	3.979e-032	1.095e-033	-31.400	-32.961	-1.560
	Fe3 (OH) 4+5	0.000e+000	0.000e+000	-41.760	-44.198	-2.438

H (0)	3.709e-012					
H2	1.855e-012	2.350e-012	-11.732	-11.629	0.103	
K	1.662e-002					
K+	1.593e-002	9.610e-003	-1.798	-2.017	-0.220	
KSO4-	6.919e-004	5.527e-004	-3.160	-3.258	-0.098	
KOH	2.329e-010	2.952e-010	-9.633	-9.530	0.103	
Mg	8.226e-002					
Mg+2	5.745e-002	1.761e-002	-1.241	-1.754	-0.514	
MgSO4	2.421e-002	3.068e-002	-1.616	-1.513	0.103	
MgHCO3+	5.932e-004	4.739e-004	-3.227	-3.324	-0.098	
MgCO3	8.775e-006	1.112e-005	-5.057	-4.954	0.103	
MgOH+	1.070e-007	8.547e-008	-6.971	-7.068	-0.098	
Mn (2)	6.189e-006					
Mn+2	3.325e-006	6.956e-007	-5.478	-6.158	-0.679	
MnCl+	1.617e-006	1.292e-006	-5.791	-5.889	-0.098	
MnSO4	7.840e-007	9.935e-007	-6.106	-6.003	0.103	
MnCl2	2.029e-007	2.572e-007	-6.693	-6.590	0.103	
MnHCO3+	1.851e-007	1.478e-007	-6.733	-6.830	-0.098	
MnCl3-	4.043e-008	3.230e-008	-7.393	-7.491	-0.098	
MnCO3	3.427e-008	4.342e-008	-7.465	-7.362	0.103	
MnOH+	7.679e-011	6.135e-011	-10.115	-10.212	-0.098	
Mn (3)	5.978e-035					
Mn+3	5.978e-035	7.922e-036	-34.223	-35.101	-0.878	
Na	7.395e-001					
Na+	7.090e-001	5.123e-001	-0.149	-0.290	-0.141	
NaSO4-	2.994e-002	2.392e-002	-1.524	-1.621	-0.098	
NaHCO3	5.422e-004	6.870e-004	-3.266	-3.163	0.103	
NaCO3-	5.218e-006	4.169e-006	-5.282	-5.380	-0.098	
NaOH	2.366e-008	2.999e-008	-7.626	-7.523	0.103	
O (0)	0.000e+000					
O2	0.000e+000	0.000e+000	-73.006	-72.903	0.103	
S (-2)	6.238e-008					
HS-	3.804e-008	2.215e-008	-7.420	-7.655	-0.235	
H2S	2.433e-008	3.083e-008	-7.614	-7.511	0.103	
Fe (HS) 2	5.895e-013	7.470e-013	-12.230	-12.127	0.103	
S-2	6.386e-014	1.099e-014	-13.195	-13.959	-0.764	
Fe (HS) 3-	2.255e-018	1.801e-018	-17.647	-17.744	-0.098	
S (6)	1.239e-001					
SO4-2	6.404e-002	1.003e-002	-1.194	-1.999	-0.805	
NaSO4-	2.994e-002	2.392e-002	-1.524	-1.621	-0.098	
MgSO4	2.421e-002	3.068e-002	-1.616	-1.513	0.103	
CaSO4	4.988e-003	6.321e-003	-2.302	-2.199	0.103	
KSO4-	6.919e-004	5.527e-004	-3.160	-3.258	-0.098	
FeSO4	1.944e-006	2.463e-006	-5.711	-5.608	0.103	
MnSO4	7.840e-007	9.935e-007	-6.106	-6.003	0.103	
HSO4-	1.060e-007	8.472e-008	-6.975	-7.072	-0.098	
CaHSO4+	4.490e-009	3.587e-009	-8.348	-8.445	-0.098	
FeHSO4+	2.179e-012	1.741e-012	-11.662	-11.759	-0.098	
FeSO4+	1.850e-020	1.478e-020	-19.733	-19.830	-0.098	
Fe (SO4) 2-	3.880e-021	3.099e-021	-20.411	-20.509	-0.098	
FeHSO4+2	1.093e-026	4.450e-027	-25.962	-26.352	-0.390	

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH)5]	-2.58	20.51	23.09	Fe2(OH)5
[Fe3(OH)7]	3.64	28.63	24.99	Fe3(OH)7
[Fe3(OH)8]	-9.23	32.89	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-21.08	37.27	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-19.00	41.38	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-14.09	29.47	43.56	Fe4(OH)8(Cl)1
Anhydrite	-0.12	-4.45	-4.33	CaSO4
Aragonite	-0.28	-8.56	-8.27	CaCO3
Brucite	-4.65	12.14	16.79	Mg(OH)2
Calcite	-0.13	-8.56	-8.43	CaCO3
CO2(g)	-1.82	-3.14	-1.32	CO2
Dolomite	0.40	-16.42	-16.82	CaMg(CO3)2
Epsomite	-1.62	-3.84	-2.22	MgSO4:7H2O
Fe(OH)2(1)	-4.81	8.13	12.94	Fe(OH)2
Fe(OH)2(2)	-5.76	8.13	13.89	Fe(OH)2
Fe(OH)3(a)	-5.81	-0.92	4.89	Fe(OH)3
FeO	-5.45	8.14	13.59	FeO
FeS(am)	-2.68	-6.46	-3.78	FeS
FeS(ppt)	-2.55	-6.46	-3.92	FeS
Goethite	-0.32	-0.90	-0.59	FeOOH
Greigite	-13.55	-52.07	-38.51	Fe3S4
Gypsum	0.11	-4.48	-4.59	CaSO4:2H2O
H2(g)	-8.53	-11.63	-3.10	H2
H2O(g)	-1.82	-0.01	1.81	H2O
H2S(g)	-6.64	-7.51	-0.87	H2S
Halite	-2.19	-0.63	1.56	NaCl
Hausmannite	-32.14	31.77	63.91	Mn3O4
Hematite	1.33	-1.80	-3.13	Fe2O3
Jarosite-H3O	-24.03	-34.56	-10.53	H3OFe3(SO4)2(OH)6
Jarosite-K	-18.92	-29.61	-10.69	KFe3(SO4)2(OH)6
Lepidocrocite	-4.31	12.39	16.70	FeOOH
Lime	-11.37	11.44	22.81	Ca(OH)2
Mackinawite	-1.92	-6.46	-4.54	FeS
Magnetite	-12.86	32.94	45.80	Fe3O4
Manganite	-13.34	12.00	25.34	MnOOH
Marcasite	5.51	-12.55	-18.06	FeS2
Melanterite	-5.50	-7.85	-2.36	FeSO4:7H2O
Nesquehonite	-2.44	-7.90	-5.46	MgCO3:3H2O
O2(g)	-70.00	-72.90	-2.91	O2
Pyrite	6.25	-12.55	-18.80	FeS2
Pyrochroite	-7.46	7.74	15.20	Mn(OH)2
Pyrolusite	-26.98	16.27	43.24	MnO2
Rhodochrosite	-1.17	-12.26	-11.09	MnCO3
Schwertmannite(1)	-46.45	-35.95	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-41.13	-23.13	18.00	Fe8O8(OH)6SO4
Siderite	-1.05	-11.87	-10.82	FeCO3
Sulfur	-4.14	1.02	5.15	S
Troilite	-0.33	-6.46	-6.13	FeS

End of simulation.

Reading input data for simulation 6.

SOLUTION 6 Dugway TW-27 (Crossgradient) 4-22-2008

temp 14.3
pH 5.49
pe 4
redox S(-2)/S(6)
units mg/kgw
density 1
S(-2) 0.065
S(6) 10900 as SO4
Ca 800
K 520
Mg 2400
Na 18000
Alkalinity 1585 as CaCO3
Fe 8.60
Mn 0.87
Cl 25600
water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 6. Dugway TW-27 (Crossgradient) 4-22-2008

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	3.167e-002	3.167e-002
Ca	1.996e-002	1.996e-002
Cl	7.221e-001	7.221e-001
Fe	1.540e-004	1.540e-004
K	1.330e-002	1.330e-002
Mg	9.872e-002	9.872e-002
Mn	1.584e-005	1.584e-005
Na	7.830e-001	7.830e-001
S(-2)	2.027e-006	2.027e-006
S(6)	1.135e-001	1.135e-001

-----Description of solution-----

pH = 5.490
pe = 4.000
Activity of water = 0.969
Ionic strength = 1.050e+000
Mass of water (kg) = 1.000e+000

Total carbon (mol/kg) = 1.356e-001
 Total CO2 (mol/kg) = 1.356e-001
 Temperature (deg C) = 14.300
 Electrical balance (eq) = 5.326e-002
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = 2.92
 Iterations = 10
 Total H = 1.110441e+002
 Total O = 5.626304e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-1.1139	-0.0635

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	4.344e-006	3.236e-006	-5.362	-5.490	-0.128
OH-	2.192e-009	1.272e-009	-8.659	-8.895	-0.236
H2O	5.551e+001	9.691e-001	1.744	-0.014	0.000
C(4)	1.356e-001				
CO2	1.040e-001	1.324e-001	-0.983	-0.878	0.105
HCO3-	2.272e-002	1.492e-002	-1.644	-1.826	-0.183
MgHCO3+	4.451e-003	3.571e-003	-2.352	-2.447	-0.096
NaHCO3	3.584e-003	4.564e-003	-2.446	-2.341	0.105
CaHCO3+	8.745e-004	5.742e-004	-3.058	-3.241	-0.183
FeHCO3+	3.407e-005	2.733e-005	-4.468	-4.563	-0.096
MnHCO3+	2.631e-006	2.111e-006	-5.580	-5.676	-0.096
MgCO3	2.274e-006	2.896e-006	-5.643	-5.538	0.105
NaCO3-	1.218e-006	9.770e-007	-5.914	-6.010	-0.096
CO3-2	9.084e-007	1.688e-007	-6.042	-6.773	-0.731
CaCO3	6.969e-007	8.876e-007	-6.157	-6.052	0.105
FeCO3	5.825e-008	7.419e-008	-7.235	-7.130	0.105
MnCO3	1.672e-008	2.129e-008	-7.777	-7.672	0.105
Fe(CO3)(OH)-	1.077e-010	8.643e-011	-9.968	-10.063	-0.096
Fe(CO3)2-2	3.551e-011	1.471e-011	-10.450	-10.832	-0.383
Ca	1.996e-002				
Ca+2	1.456e-002	3.706e-003	-1.837	-2.431	-0.594
CaSO4	4.524e-003	5.761e-003	-2.344	-2.239	0.105
CaHCO3+	8.745e-004	5.742e-004	-3.058	-3.241	-0.183
CaCO3	6.969e-007	8.876e-007	-6.157	-6.052	0.105
CaHSO4+	1.208e-007	9.695e-008	-6.918	-7.013	-0.096
CaOH+	2.296e-010	1.842e-010	-9.639	-9.735	-0.096
Cl	7.221e-001				
Cl-	7.221e-001	4.346e-001	-0.141	-0.362	-0.220
FeCl+	1.370e-005	1.099e-005	-4.863	-4.959	-0.096
MnCl+	3.504e-006	2.811e-006	-5.455	-5.551	-0.096
MnCl2	4.187e-007	5.332e-007	-6.378	-6.273	0.105
MnCl3-	7.955e-008	6.383e-008	-7.099	-7.195	-0.096
FeCl2+	2.327e-018	1.867e-018	-17.633	-17.729	-0.096
FeCl+2	1.633e-018	6.765e-019	-17.787	-18.170	-0.383

FeCl3	6.371e-020	8.113e-020	-19.196	-19.091	0.105
Fe (2)	1.540e-004				
Fe+2	8.812e-005	1.832e-005	-4.055	-4.737	-0.682
FeHCO3+	3.407e-005	2.733e-005	-4.468	-4.563	-0.096
FeSO4	1.805e-005	2.298e-005	-4.744	-4.639	0.105
FeCl+	1.370e-005	1.099e-005	-4.863	-4.959	-0.096
FeCO3	5.825e-008	7.419e-008	-7.235	-7.130	0.105
FeOH+	9.437e-010	7.571e-010	-9.025	-9.121	-0.096
FeHSO4+	5.974e-010	4.793e-010	-9.224	-9.319	-0.096
Fe (CO3) (OH) -	1.077e-010	8.643e-011	-9.968	-10.063	-0.096
Fe (HS) 2	4.723e-011	6.014e-011	-10.326	-10.221	0.105
Fe (CO3) 2-2	3.551e-011	1.471e-011	-10.450	-10.832	-0.383
Fe (OH) 2	3.167e-015	4.033e-015	-14.499	-14.394	0.105
Fe (HS) 3-	4.954e-016	3.975e-016	-15.305	-15.401	-0.096
Fe (3)	6.261e-015				
Fe (OH) 2+	5.981e-015	4.798e-015	-14.223	-14.319	-0.096
FeOH+2	1.779e-016	7.371e-017	-15.750	-16.132	-0.383
Fe (OH) 3	8.961e-017	1.141e-016	-16.048	-15.943	0.105
FeSO4+	6.769e-018	5.431e-018	-17.169	-17.265	-0.096
FeCl2+	2.327e-018	1.867e-018	-17.633	-17.729	-0.096
FeCl+2	1.633e-018	6.765e-019	-17.787	-18.170	-0.383
Fe (SO4) 2-	1.226e-018	9.832e-019	-17.912	-18.007	-0.096
Fe+3	1.037e-018	7.327e-020	-17.984	-19.135	-1.151
FeCl3	6.371e-020	8.113e-020	-19.196	-19.091	0.105
Fe (OH) 4-	2.487e-020	1.995e-020	-19.604	-19.700	-0.096
FeHSO4+2	1.162e-022	4.815e-023	-21.935	-22.317	-0.383
Fe2 (OH) 2+4	7.851e-030	2.314e-031	-29.105	-30.636	-1.531
Fe3 (OH) 4+5	1.591e-040	0.000e+000	-39.798	-42.190	-2.392
H (0)	2.197e-012				
H2	1.098e-012	1.399e-012	-11.959	-11.854	0.105
K	1.330e-002				
K+	1.282e-002	7.714e-003	-1.892	-2.113	-0.220
KSO4-	4.811e-004	3.860e-004	-3.318	-3.413	-0.096
KOH	6.290e-012	8.011e-012	-11.201	-11.096	0.105
Mg	9.872e-002				
Mg+2	6.894e-002	2.119e-002	-1.162	-1.674	-0.512
MgSO4	2.533e-002	3.226e-002	-1.596	-1.491	0.105
MgHCO3+	4.451e-003	3.571e-003	-2.352	-2.447	-0.096
MgCO3	2.274e-006	2.896e-006	-5.643	-5.538	0.105
MgOH+	4.549e-009	3.650e-009	-8.342	-8.438	-0.096
Mn (2)	1.584e-005				
Mn+2	7.636e-006	1.588e-006	-5.117	-5.799	-0.682
MnCl+	3.504e-006	2.811e-006	-5.455	-5.551	-0.096
MnHCO3+	2.631e-006	2.111e-006	-5.580	-5.676	-0.096
MnSO4	1.550e-006	1.974e-006	-5.810	-5.705	0.105
MnCl2	4.187e-007	5.332e-007	-6.378	-6.273	0.105
MnCl3-	7.955e-008	6.383e-008	-7.099	-7.195	-0.096
MnCO3	1.672e-008	2.129e-008	-7.777	-7.672	0.105
MnOH+	6.164e-012	4.946e-012	-11.210	-11.306	-0.096
Mn (3)	5.419e-033				
Mn+3	5.419e-033	7.463e-034	-32.266	-33.127	-0.861
Na	7.830e-001				
Na+	7.520e-001	5.440e-001	-0.124	-0.264	-0.141
NaSO4-	2.737e-002	2.196e-002	-1.563	-1.658	-0.096

NaHCO3	3.584e-003	4.564e-003	-2.446	-2.341	0.105
NaCO3-	1.218e-006	9.770e-007	-5.914	-6.010	-0.096
NaOH	8.452e-010	1.076e-009	-9.073	-8.968	0.105
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-72.385	-72.280	0.105
S (-2)	2.027e-006				
H2S	1.923e-006	2.448e-006	-5.716	-5.611	0.105
HS-	1.046e-007	6.069e-008	-6.981	-7.217	-0.236
Fe (HS) 2	4.723e-011	6.014e-011	-10.326	-10.221	0.105
S-2	6.202e-015	1.059e-015	-14.207	-14.975	-0.768
Fe (HS) 3-	4.954e-016	3.975e-016	-15.305	-15.401	-0.096
S (6)	1.135e-001				
SO4-2	5.574e-002	8.642e-003	-1.254	-2.063	-0.810
NaSO4-	2.737e-002	2.196e-002	-1.563	-1.658	-0.096
MgSO4	2.533e-002	3.226e-002	-1.596	-1.491	0.105
CaSO4	4.524e-003	5.761e-003	-2.344	-2.239	0.105
KSO4-	4.811e-004	3.860e-004	-3.318	-3.413	-0.096
FeSO4	1.805e-005	2.298e-005	-4.744	-4.639	0.105
HSO4-	2.712e-006	2.176e-006	-5.567	-5.662	-0.096
MnSO4	1.550e-006	1.974e-006	-5.810	-5.705	0.105
CaHSO4+	1.208e-007	9.695e-008	-6.918	-7.013	-0.096
FeHSO4+	5.974e-010	4.793e-010	-9.224	-9.319	-0.096
FeSO4+	6.769e-018	5.431e-018	-17.169	-17.265	-0.096
Fe (SO4) 2-	1.226e-018	9.832e-019	-17.912	-18.007	-0.096
FeHSO4+2	1.162e-022	4.815e-023	-21.935	-22.317	-0.383

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH) 5]	-6.30	16.79	23.09	Fe2(OH) 5
[Fe3(OH) 7]	-1.98	23.01	24.99	Fe3(OH) 7
[Fe3(OH) 8]	-14.75	27.37	42.12	Fe3(OH) 8
[Fe6(OH) 12] [CO3]	-30.06	28.29	58.35	Fe6(OH) 12 (CO3) 1
[Fe6(OH) 12] [SO4]	-27.38	33.00	60.38	Fe6(OH) 12 (SO4) 1
[Fe6(OH) 8] [Cl]	-20.17	23.39	43.56	Fe4(OH) 8 (Cl) 1
Anhydrite	-0.16	-4.49	-4.33	CaSO4
Aragonite	-0.93	-9.20	-8.28	CaCO3
Brucite	-7.51	9.28	16.79	Mg (OH) 2
Calcite	-0.78	-9.20	-8.43	CaCO3
CO2 (g)	0.45	-0.88	-1.33	CO2
Dolomite	-0.82	-17.65	-16.83	CaMg (CO3) 2
Epsomite	-1.62	-3.83	-2.22	MgSO4:7H2O
Fe (OH) 2 (1)	-6.72	6.22	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-7.67	6.22	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-7.60	-2.71	4.89	Fe (OH) 3
FeO	-7.36	6.23	13.59	FeO
FeS (am)	-2.68	-6.46	-3.79	FeS
FeS (ppt)	-2.55	-6.46	-3.92	FeS
Goethite	-2.09	-2.69	-0.60	FeOOH
Greigite	-11.39	-49.91	-38.53	Fe3S4
Gypsum	0.06	-4.52	-4.59	CaSO4:2H2O
H2 (g)	-8.75	-11.85	-3.10	H2
H2O (g)	-1.81	-0.01	1.80	H2O

H2S(g)	-4.74	-5.61	-0.87	H2S
Halite	-2.18	-0.63	1.56	NaCl
Hausmannite	-39.54	24.24	63.78	Mn3O4
Hematite	-2.20	-5.37	-3.17	Fe2O3
Jarosite-H3O	-23.57	-34.18	-10.61	H3OFe3(SO4)2(OH)6
Jarosite-K	-20.08	-30.79	-10.71	KFe3(SO4)2(OH)6
Lepidocrocite	-6.11	10.59	16.70	FeOOH
Lime	-14.29	8.52	22.81	Ca(OH)2
Mackinawite	-1.92	-6.46	-4.54	FeS
Magnetite	-18.37	27.43	45.80	Fe3O4
Manganite	-15.81	9.53	25.34	MnOOH
Marcasite	7.63	-10.42	-18.04	FeS2
Melanterite	-4.55	-6.90	-2.35	FeSO4·7H2O
Nesquehonite	-3.02	-8.49	-5.46	MgCO3·3H2O
O2(g)	-69.37	-72.28	-2.91	O2
Pyrite	8.37	-10.42	-18.79	FeS2
Pyrochroite	-10.05	5.15	15.20	Mn(OH)2
Pyrolusite	-29.25	13.91	43.16	MnO2
Rhodochrosite	-1.48	-12.57	-11.09	MnCO3
Schwertmannite(1)	-55.58	-45.08	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-52.55	-34.55	18.00	Fe8O8(OH)6SO4
Siderite	-0.69	-11.51	-10.82	FeCO3
Sulfur	-2.00	3.14	5.14	S
Troilite	-0.33	-6.46	-6.13	FeS

End of simulation.

Reading input data for simulation 7.

SOLUTION 7 Dugway TW-28 (Injection Zone) 4-22-2008

temp	13.9
pH	6.30
pe	4
redox	S(-2)/S(6)
units	mg/kgw
density	1
S(-2)	1.045
S(6)	10400 as SO4
Ca	740
K	530
Mg	1900
Na	16000
Alkalinity	2341 as CaCO3
Fe	4.10
Mn	1.3
Cl	24700
water	1 # kg

END

Beginning of initial solution calculations.

Initial solution 7. Dugway TW-28 (Injection Zone) 4-22-2008

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	4.678e-002	4.678e-002
Ca	1.846e-002	1.846e-002
Cl	6.967e-001	6.967e-001
Fe	7.341e-005	7.341e-005
K	1.355e-002	1.355e-002
Mg	7.815e-002	7.815e-002
Mn	2.366e-005	2.366e-005
Na	6.960e-001	6.960e-001
S(-2)	3.259e-005	3.259e-005
S(6)	1.083e-001	1.083e-001

-----Description of solution-----

pH	=	6.300
pe	=	4.000
Activity of water	=	0.972
Ionic strength	=	9.666e-001
Mass of water (kg)	=	1.000e+000
Total carbon (mol/kg)	=	7.241e-002
Total CO2 (mol/kg)	=	7.241e-002
Temperature (deg C)	=	13.900
Electrical balance (eq)	=	-5.706e-002
Percent error, 100*(Cat- An)/(Cat+ An)	=	-3.38
Iterations	=	10
Total H	=	1.110592e+002
Total O	=	5.613080e+001

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-2.2516	-0.1282

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	6.706e-007	5.012e-007	-6.174	-6.300	-0.126
OH-	1.358e-008	7.968e-009	-7.867	-8.099	-0.232
H2O	5.551e+001	9.724e-001	1.744	-0.012	0.000
C(4)	7.241e-002				
HCO3-	3.517e-002	2.324e-002	-1.454	-1.634	-0.180
CO2	2.568e-002	3.208e-002	-1.590	-1.494	0.097

	MgHCO3+	5.292e-003	4.175e-003	-2.276	-2.379	-0.103
	NaHCO3	5.007e-003	6.255e-003	-2.300	-2.204	0.097
	CaHCO3+	1.188e-003	7.851e-004	-2.925	-3.105	-0.180
	FeHCO3+	2.278e-005	1.797e-005	-4.643	-4.745	-0.103
	MgCO3	1.722e-005	2.152e-005	-4.764	-4.667	0.097
	NaCO3-	1.061e-005	8.370e-006	-4.974	-5.077	-0.103
	CO3-2	8.811e-006	1.680e-006	-5.055	-5.775	-0.720
	CaCO3	6.239e-006	7.794e-006	-5.205	-5.108	0.097
	MnHCO3+	5.665e-006	4.469e-006	-5.247	-5.350	-0.103
	FeCO3	2.494e-007	3.116e-007	-6.603	-6.506	0.097
	MnCO3	2.305e-007	2.879e-007	-6.637	-6.541	0.097
	Fe (CO3) (OH) -	2.981e-009	2.352e-009	-8.526	-8.629	-0.103
	Fe (CO3) 2-2	1.588e-009	6.150e-010	-8.799	-9.211	-0.412
Ca		1.846e-002				
	Ca+2	1.295e-002	3.284e-003	-1.888	-2.484	-0.596
	CaSO4	4.322e-003	5.400e-003	-2.364	-2.268	0.097
	CaHCO3+	1.188e-003	7.851e-004	-2.925	-3.105	-0.180
	CaCO3	6.239e-006	7.794e-006	-5.205	-5.108	0.097
	CaHSO4+	1.777e-008	1.402e-008	-7.750	-7.853	-0.103
	CaOH+	1.340e-009	1.058e-009	-8.873	-8.976	-0.103
Cl		6.967e-001				
	Cl-	6.967e-001	4.226e-001	-0.157	-0.374	-0.217
	FeCl+	5.717e-006	4.510e-006	-5.243	-5.346	-0.103
	MnCl+	4.709e-006	3.715e-006	-5.327	-5.430	-0.103
	MnCl2	5.485e-007	6.852e-007	-6.261	-6.164	0.097
	MnCl3-	1.011e-007	7.976e-008	-6.995	-7.098	-0.103
	FeCl2+	6.716e-020	5.299e-020	-19.173	-19.276	-0.103
	FeCl+2	5.028e-020	1.948e-020	-19.299	-19.710	-0.412
	FeCl3	1.792e-021	2.239e-021	-20.747	-20.650	0.097
Fe (2)		7.341e-005				
	Fe+2	3.636e-005	7.732e-006	-4.439	-5.112	-0.672
	FeHCO3+	2.278e-005	1.797e-005	-4.643	-4.745	-0.103
	FeSO4	8.181e-006	1.022e-005	-5.087	-4.991	0.097
	FeCl+	5.717e-006	4.510e-006	-5.243	-5.346	-0.103
	FeCO3	2.494e-007	3.116e-007	-6.603	-6.506	0.097
	Fe (HS) 2	1.255e-007	1.568e-007	-6.901	-6.805	0.097
	Fe (CO3) (OH) -	2.981e-009	2.352e-009	-8.526	-8.629	-0.103
	FeOH+	2.541e-009	2.004e-009	-8.595	-8.698	-0.103
	Fe (CO3) 2-2	1.588e-009	6.150e-010	-8.799	-9.211	-0.412
	Fe (HS) 3-	1.032e-010	8.144e-011	-9.986	-10.089	-0.103
	FeHSO4+	4.184e-011	3.301e-011	-10.378	-10.481	-0.103
	Fe (OH) 2	5.719e-014	7.145e-014	-13.243	-13.146	0.097
Fe (3)		8.091e-015				
	Fe (OH) 2+	7.351e-015	5.799e-015	-14.134	-14.237	-0.103
	Fe (OH) 3	7.020e-016	8.770e-016	-15.154	-15.057	0.097
	FeOH+2	3.608e-017	1.398e-017	-16.443	-16.855	-0.412
	Fe (OH) 4-	1.238e-018	9.764e-019	-17.907	-18.010	-0.103
	FeSO4+	2.174e-019	1.715e-019	-18.663	-18.766	-0.103
	FeCl2+	6.716e-020	5.299e-020	-19.173	-19.276	-0.103
	FeCl+2	5.028e-020	1.948e-020	-19.299	-19.710	-0.412
	Fe (SO4) 2-	4.172e-020	3.291e-020	-19.380	-19.483	-0.103
	Fe+3	3.023e-020	2.200e-021	-19.520	-20.658	-1.138
	FeCl3	1.792e-021	2.239e-021	-20.747	-20.650	0.097
	FeHSO4+2	6.088e-025	2.359e-025	-24.216	-24.627	-0.412

Fe2 (OH) 2+4	3.759e-031	8.467e-033	-30.425	-32.072	-1.647
Fe3 (OH) 4+5	0.000e+000	0.000e+000	-40.953	-43.527	-2.574
H (0)	1.017e-011				
H2	5.086e-012	6.354e-012	-11.294	-11.197	0.097
K	1.355e-002				
K+	1.303e-002	7.901e-003	-1.885	-2.102	-0.217
KSO4-	5.281e-004	4.167e-004	-3.277	-3.380	-0.103
KOH	4.255e-011	5.316e-011	-10.371	-10.274	0.097
Mg	7.815e-002				
Mg+2	5.247e-002	1.592e-002	-1.280	-1.798	-0.518
MgSO4	2.037e-002	2.545e-002	-1.691	-1.594	0.097
MgHCO3+	5.292e-003	4.175e-003	-2.276	-2.379	-0.103
MgCO3	1.722e-005	2.152e-005	-4.764	-4.667	0.097
MgOH+	2.166e-008	1.708e-008	-7.664	-7.767	-0.103
Mn (2)	2.366e-005				
Mn+2	1.015e-005	2.158e-006	-4.994	-5.666	-0.672
MnHCO3+	5.665e-006	4.469e-006	-5.247	-5.350	-0.103
MnCl+	4.709e-006	3.715e-006	-5.327	-5.430	-0.103
MnSO4	2.262e-006	2.826e-006	-5.645	-5.549	0.097
MnCl2	5.485e-007	6.852e-007	-6.261	-6.164	0.097
MnCO3	2.305e-007	2.879e-007	-6.637	-6.541	0.097
MnCl3-	1.011e-007	7.976e-008	-6.995	-7.098	-0.103
MnOH+	5.329e-011	4.205e-011	-10.273	-10.376	-0.103
Mn (3)	5.859e-034				
Mn+3	5.859e-034	6.937e-035	-33.232	-34.159	-0.927
Na	6.960e-001				
Na+	6.650e-001	4.786e-001	-0.177	-0.320	-0.143
NaSO4-	2.594e-002	2.046e-002	-1.586	-1.689	-0.103
NaHCO3	5.007e-003	6.255e-003	-2.300	-2.204	0.097
NaCO3-	1.061e-005	8.370e-006	-4.974	-5.077	-0.103
NaOH	4.911e-009	6.135e-009	-8.309	-8.212	0.097
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-73.828	-73.731	0.097
S (-2)	3.259e-005				
H2S	2.421e-005	3.024e-005	-4.616	-4.519	0.097
HS-	8.131e-006	4.770e-006	-5.090	-5.321	-0.232
Fe (HS) 2	1.255e-007	1.568e-007	-6.901	-6.805	0.097
Fe (HS) 3-	1.032e-010	8.144e-011	-9.986	-10.089	-0.103
S-2	2.970e-012	5.219e-013	-11.527	-12.282	-0.755
S (6)	1.083e-001				
SO4-2	5.709e-002	9.177e-003	-1.243	-2.037	-0.794
NaSO4-	2.594e-002	2.046e-002	-1.586	-1.689	-0.103
MgSO4	2.037e-002	2.545e-002	-1.691	-1.594	0.097
CaSO4	4.322e-003	5.400e-003	-2.364	-2.268	0.097
KSO4-	5.281e-004	4.167e-004	-3.277	-3.380	-0.103
FeSO4	8.181e-006	1.022e-005	-5.087	-4.991	0.097
MnSO4	2.262e-006	2.826e-006	-5.645	-5.549	0.097
HSO4-	4.501e-007	3.551e-007	-6.347	-6.450	-0.103
CaHSO4+	1.777e-008	1.402e-008	-7.750	-7.853	-0.103
FeHSO4+	4.184e-011	3.301e-011	-10.378	-10.481	-0.103
FeSO4+	2.174e-019	1.715e-019	-18.663	-18.766	-0.103
Fe (SO4) 2-	4.172e-020	3.291e-020	-19.380	-19.483	-0.103
FeHSO4+2	6.088e-025	2.359e-025	-24.216	-24.627	-0.412

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH)5]	-4.13	18.96	23.09	Fe2(OH)5
[Fe3(OH)7]	1.44	26.43	24.99	Fe3(OH)7
[Fe3(OH)8]	-11.66	30.46	42.12	Fe3(OH)8
[Fe6(OH)12][CO3]	-23.84	34.51	58.35	Fe6(OH)12(CO3)1
[Fe6(OH)12][SO4]	-22.14	38.24	60.38	Fe6(OH)12(SO4)1
[Fe6(OH)8][Cl]	-16.33	27.23	43.56	Fe4(OH)8(Cl)1
Anhydrite	-0.19	-4.52	-4.33	CaSO4
Aragonite	0.02	-8.26	-8.27	CaCO3
Brucite	-6.01	10.78	16.79	Mg(OH)2
Calcite	0.17	-8.26	-8.43	CaCO3
CO2(g)	-0.17	-1.49	-1.33	CO2
Dolomite	0.99	-15.83	-16.82	CaMg(CO3)2
Epsomite	-1.70	-3.92	-2.22	MgSO4·7H2O
Fe(OH)2(1)	-5.48	7.46	12.94	Fe(OH)2
Fe(OH)2(2)	-6.43	7.46	13.89	Fe(OH)2
Fe(OH)3(a)	-6.69	-1.79	4.89	Fe(OH)3
FeO	-6.11	7.48	13.59	FeO
FeS(am)	-0.35	-4.13	-3.78	FeS
FeS(ppt)	-0.22	-4.13	-3.92	FeS
Goethite	-1.19	-1.78	-0.59	FeOOH
Greigite	-4.00	-42.51	-38.52	Fe3S4
Gypsum	0.04	-4.55	-4.59	CaSO4·2H2O
H2(g)	-8.10	-11.20	-3.10	H2
H2O(g)	-1.82	-0.01	1.81	H2O
H2S(g)	-3.65	-4.52	-0.87	H2S
Halite	-2.25	-0.69	1.56	NaCl
Hausmannite	-35.03	28.85	63.88	Mn3O4
Hematite	-0.42	-3.55	-3.13	Fe2O3
Jarosite-H3O	-24.09	-34.63	-10.55	H3OFe3(SO4)2(OH)6
Jarosite-K	-19.73	-30.42	-10.70	KFe3(SO4)2(OH)6
Lepidocrocite	-5.19	11.51	16.70	FeOOH
Lime	-12.72	10.09	22.81	Ca(OH)2
Mackinawite	0.41	-4.13	-4.54	FeS
Magnetite	-15.29	30.51	45.80	Fe3O4
Manganite	-14.38	10.96	25.34	MnOOH
Marcasite	10.40	-7.66	-18.06	FeS2
Melanterite	-4.88	-7.23	-2.35	FeSO4·7H2O
Nesquehonite	-2.15	-7.61	-5.46	MgCO3·3H2O
O2(g)	-70.82	-73.73	-2.91	O2
Pyrite	11.14	-7.66	-18.80	FeS2
Pyrochroite	-8.29	6.91	15.20	Mn(OH)2
Pyrolusite	-28.22	15.01	43.23	MnO2
Rhodochrosite	-0.35	-11.44	-11.09	MnCO3
Schwertmannite(1)	-51.16	-40.66	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-46.87	-28.87	18.00	Fe8O8(OH)6SO4
Siderite	-0.07	-10.89	-10.82	FeCO3
Sulfur	-1.57	3.58	5.15	S
Troilite	1.99	-4.13	-6.13	FeS

End of simulation.

Reading input data for simulation 8.

SOLUTION 8 Dugway TW-29 (Downgradient) 4-22-2008

temp 13.7
pH 5.44
pe 4
redox S(-2)/S(6)
units mg/kgw
density 1
S(-2) 0.083
S(6) 10800 as SO4
Ca 760
K 500
Mg 2200
Na 16000
Alkalinity 1896 as CaCO3
Fe 18.0
Mn 1.2
Cl 25900
water 1 # kg

END

Beginning of initial solution calculations.

Initial solution 8. Dugway TW-29 (Downgradient) 4-22-2008

WARNING: Equivalent wt for alkalinity should be Ca.5(CO3).5. Using 50.0455 g/eq.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	3.789e-002	3.789e-002
Ca	1.896e-002	1.896e-002
Cl	7.305e-001	7.305e-001
Fe	3.223e-004	3.223e-004
K	1.279e-002	1.279e-002
Mg	9.049e-002	9.049e-002
Mn	2.184e-005	2.184e-005
Na	6.960e-001	6.960e-001
S(-2)	2.589e-006	2.589e-006
S(6)	1.124e-001	1.124e-001

-----Description of solution-----

pH = 5.440
pe = 4.000
Activity of water = 0.970

```

          Ionic strength = 1.001e+000
        Mass of water (kg) = 1.000e+000
      Total carbon (mol/kg) = 1.851e-001
        Total CO2 (mol/kg) = 1.851e-001
        Temperature (deg C) = 13.700
      Electrical balance (eq) = -6.494e-002
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -3.74
          Iterations = 10
            Total H = 1.110503e+002
            Total O = 5.636398e+001

```

-----Redox couples-----

Redox couple	pe	Eh (volts)
S(-2)/S(6)	-1.0482	-0.0597

-----Distribution of species-----

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma
H+	4.864e-006	3.631e-006	-5.313	-5.440	-0.127
OH-	1.846e-009	1.078e-009	-8.734	-8.967	-0.233
H2O	5.551e+001	9.697e-001	1.744	-0.013	0.000
C(4)	1.851e-001				
CO2	1.472e-001	1.854e-001	-0.832	-0.732	0.100
HCO3-	2.793e-002	1.841e-002	-1.554	-1.735	-0.181
MgHCO3+	4.930e-003	3.916e-003	-2.307	-2.407	-0.100
NaHCO3	3.951e-003	4.975e-003	-2.403	-2.303	0.100
CaHCO3+	9.818e-004	6.471e-004	-3.008	-3.189	-0.181
FeHCO3+	8.413e-005	6.684e-005	-4.075	-4.175	-0.100
MnHCO3+	4.317e-006	3.430e-006	-5.365	-5.465	-0.100
MgCO3	2.195e-006	2.764e-006	-5.659	-5.558	0.100
NaCO3-	1.138e-006	9.043e-007	-5.944	-6.044	-0.100
CO3-2	9.683e-007	1.827e-007	-6.014	-6.738	-0.724
CaCO3	7.024e-007	8.846e-007	-6.153	-6.053	0.100
FeCO3	1.264e-007	1.592e-007	-6.898	-6.798	0.100
MnCO3	2.409e-008	3.034e-008	-7.618	-7.518	0.100
Fe(CO3)(OH)-	2.082e-010	1.654e-010	-9.682	-9.782	-0.100
Fe(CO3)2-2	8.577e-011	3.417e-011	-10.067	-10.466	-0.400
Ca	1.896e-002				
Ca+2	1.351e-002	3.434e-003	-1.869	-2.464	-0.595
CaSO4	4.469e-003	5.627e-003	-2.350	-2.250	0.100
CaHCO3+	9.818e-004	6.471e-004	-3.008	-3.189	-0.181
CaCO3	7.024e-007	8.846e-007	-6.153	-6.053	0.100
CaHSO4+	1.330e-007	1.056e-007	-6.876	-6.976	-0.100
CaOH+	1.916e-010	1.522e-010	-9.718	-9.818	-0.100
Cl	7.305e-001				
Cl-	7.305e-001	4.417e-001	-0.136	-0.355	-0.218
FeCl+	2.787e-005	2.214e-005	-4.555	-4.655	-0.100
MnCl+	4.735e-006	3.761e-006	-5.325	-5.425	-0.100
MnCl2	5.760e-007	7.253e-007	-6.240	-6.139	0.100
MnCl3-	1.111e-007	8.824e-008	-6.954	-7.054	-0.100

FeCl ₂ +	5.401e-018	4.291e-018	-17.268	-17.367	-0.100
FeCl+2	3.762e-018	1.499e-018	-17.425	-17.824	-0.400
FeCl ₃	1.505e-019	1.896e-019	-18.822	-18.722	0.100
Fe (2)	3.223e-004				
Fe+2	1.723e-004	3.631e-005	-3.764	-4.440	-0.676
FeHCO ₃ +	8.413e-005	6.684e-005	-4.075	-4.175	-0.100
FeSO ₄	3.791e-005	4.774e-005	-4.421	-4.321	0.100
FeCl+	2.787e-005	2.214e-005	-4.555	-4.655	-0.100
FeCO ₃	1.264e-007	1.592e-007	-6.898	-6.798	0.100
FeOH+	1.605e-009	1.275e-009	-8.795	-8.895	-0.100
FeHSO ₄ +	1.406e-009	1.117e-009	-8.852	-8.952	-0.100
Fe (CO ₃) (OH) -	2.082e-010	1.654e-010	-9.682	-9.782	-0.100
Fe (HS) 2	1.164e-010	1.466e-010	-9.934	-9.834	0.100
Fe (CO ₃) 2-2	8.577e-011	3.417e-011	-10.067	-10.466	-0.400
Fe (OH) 2	5.048e-015	6.357e-015	-14.297	-14.197	0.100
Fe (HS) 3-	1.352e-015	1.074e-015	-14.869	-14.969	-0.100
Fe (3)	1.055e-014				
Fe (OH) 2+	1.004e-014	7.975e-015	-13.998	-14.098	-0.100
FeOH+2	3.534e-016	1.408e-016	-15.452	-15.851	-0.400
Fe (OH) 3	1.306e-016	1.645e-016	-15.884	-15.784	0.100
FeSO ₄ +	1.590e-017	1.263e-017	-16.799	-16.898	-0.100
FeCl ₂ +	5.401e-018	4.291e-018	-17.268	-17.367	-0.100
FeCl+2	3.762e-018	1.499e-018	-17.425	-17.824	-0.400
Fe (SO ₄) 2-	3.046e-018	2.420e-018	-17.516	-17.616	-0.100
Fe+3	2.266e-018	1.630e-019	-17.645	-18.788	-1.143
FeCl ₃	1.505e-019	1.896e-019	-18.822	-18.722	0.100
Fe (OH) 4-	3.145e-020	2.499e-020	-19.502	-19.602	-0.100
FeHSO ₄ +2	3.162e-022	1.260e-022	-21.500	-21.900	-0.400
Fe ₂ (OH) 2+4	3.442e-029	8.668e-031	-28.463	-30.062	-1.599
Fe ₃ (OH) 4+5	1.344e-039	0.000e+000	-38.871	-41.370	-2.498
H (0)	2.081e-012				
H ₂	1.040e-012	1.310e-012	-11.983	-11.883	0.100
K	1.279e-002				
K+	1.230e-002	7.435e-003	-1.910	-2.129	-0.218
KSO ₄ -	4.911e-004	3.901e-004	-3.309	-3.409	-0.100
KOH	5.468e-012	6.886e-012	-11.262	-11.162	0.100
Mg	9.049e-002				
Mg+2	6.179e-002	1.886e-002	-1.209	-1.725	-0.515
MgSO ₄	2.377e-002	2.994e-002	-1.624	-1.524	0.100
MgHCO ₃ +	4.930e-003	3.916e-003	-2.307	-2.407	-0.100
MgCO ₃	2.195e-006	2.764e-006	-5.659	-5.558	0.100
MgOH+	3.439e-009	2.732e-009	-8.464	-8.564	-0.100
Mn (2)	2.184e-005				
Mn+2	9.918e-006	2.090e-006	-5.004	-5.680	-0.676
MnCl+	4.735e-006	3.761e-006	-5.325	-5.425	-0.100
MnHCO ₃ +	4.317e-006	3.430e-006	-5.365	-5.465	-0.100
MnSO ₄	2.162e-006	2.723e-006	-5.665	-5.565	0.100
MnCl ₂	5.760e-007	7.253e-007	-6.240	-6.139	0.100
MnCl ₃ -	1.111e-007	8.824e-008	-6.954	-7.054	-0.100
MnCO ₃	2.409e-008	3.034e-008	-7.618	-7.518	0.100
MnOH+	6.934e-012	5.509e-012	-11.159	-11.259	-0.100
Mn (3)	8.247e-033				
Mn+3	8.247e-033	1.040e-033	-32.084	-32.983	-0.899
Na	6.960e-001				

Na+	6.662e-001	4.806e-001	-0.176	-0.318	-0.142
NaSO4-	2.579e-002	2.049e-002	-1.588	-1.688	-0.100
NaHCO3	3.951e-003	4.975e-003	-2.403	-2.303	0.100
NaCO3-	1.138e-006	9.043e-007	-5.944	-6.044	-0.100
NaOH	6.734e-010	8.480e-010	-9.172	-9.072	0.100
O (0)	0.000e+000				
O2	0.000e+000	0.000e+000	-72.532	-72.432	0.100
S (-2)	2.589e-006				
H2S	2.473e-006	3.114e-006	-5.607	-5.507	0.100
HS-	1.152e-007	6.731e-008	-6.938	-7.172	-0.233
Fe (HS) 2	1.164e-010	1.466e-010	-9.934	-9.834	0.100
S-2	5.765e-015	1.002e-015	-14.239	-14.999	-0.760
Fe (HS) 3-	1.352e-015	1.074e-015	-14.869	-14.969	-0.100
S (6)	1.124e-001				
SO4-2	5.786e-002	9.166e-003	-1.238	-2.038	-0.800
NaSO4-	2.579e-002	2.049e-002	-1.588	-1.688	-0.100
MgSO4	2.377e-002	2.994e-002	-1.624	-1.524	0.100
CaSO4	4.469e-003	5.627e-003	-2.350	-2.250	0.100
KSO4-	4.911e-004	3.901e-004	-3.309	-3.409	-0.100
FeSO4	3.791e-005	4.774e-005	-4.421	-4.321	0.100
HSO4-	3.221e-006	2.559e-006	-5.492	-5.592	-0.100
MnSO4	2.162e-006	2.723e-006	-5.665	-5.565	0.100
CaHSO4+	1.330e-007	1.056e-007	-6.876	-6.976	-0.100
FeHSO4+	1.406e-009	1.117e-009	-8.852	-8.952	-0.100
FeSO4+	1.590e-017	1.263e-017	-16.799	-16.898	-0.100
Fe (SO4) 2-	3.046e-018	2.420e-018	-17.516	-17.616	-0.100
FeHSO4+2	3.162e-022	1.260e-022	-21.500	-21.900	-0.400

-----Saturation indices-----

Phase	SI	log IAP	log KT	
[Fe2(OH) 5]	-5.89	17.20	23.09	Fe2(OH) 5
[Fe3(OH) 7]	-1.37	23.62	24.99	Fe3(OH) 7
[Fe3(OH) 8]	-14.12	28.00	42.12	Fe3(OH) 8
[Fe6(OH) 12] [CO3]	-28.71	29.64	58.35	Fe6(OH) 12 (CO3) 1
[Fe6(OH) 12] [SO4]	-26.03	34.35	60.38	Fe6(OH) 12 (SO4) 1
[Fe6(OH) 8] [Cl]	-19.31	24.25	43.56	Fe4(OH) 8 (Cl) 1
Anhydrite	-0.17	-4.50	-4.33	CaSO4
Aragonite	-0.93	-9.20	-8.27	CaCO3
Brucite	-7.66	9.13	16.79	Mg (OH) 2
Calcite	-0.78	-9.20	-8.42	CaCO3
CO2 (g)	0.59	-0.73	-1.32	CO2
Dolomite	-0.85	-17.67	-16.82	CaMg (CO3) 2
Epsomite	-1.63	-3.86	-2.22	MgSO4:7H2O
Fe (OH) 2 (1)	-6.53	6.41	12.94	Fe (OH) 2
Fe (OH) 2 (2)	-7.48	6.41	13.89	Fe (OH) 2
Fe (OH) 3 (a)	-7.40	-2.51	4.89	Fe (OH) 3
FeO	-7.16	6.43	13.59	FeO
FeS (am)	-2.39	-6.17	-3.78	FeS
FeS (ppt)	-2.26	-6.17	-3.92	FeS
Goethite	-1.91	-2.49	-0.58	FeOOH
Greigite	-10.43	-48.94	-38.51	Fe3S4
Gypsum	0.06	-4.53	-4.59	CaSO4:2H2O

H2(g)	-8.78	-11.88	-3.10	H2
H2O(g)	-1.83	-0.01	1.81	H2O
H2S(g)	-4.64	-5.51	-0.87	H2S
Halite	-2.23	-0.67	1.56	NaCl
Hausmannite	-39.61	24.33	63.94	Mn3O4
Hematite	-1.86	-4.98	-3.12	Fe2O3
Jarosite-H3O	-22.81	-33.33	-10.52	H3OFe3(SO4)2(OH)6
Jarosite-K	-19.32	-30.01	-10.69	KFe3(SO4)2(OH)6
Lepidocrocite	-5.89	10.81	16.70	FeOOH
Lime	-14.42	8.39	22.81	Ca(OH)2
Mackinawite	-1.63	-6.17	-4.54	FeS
Magnetite	-17.75	28.05	45.80	Fe3O4
Manganite	-15.77	9.57	25.34	MnOOH
Marcasite	8.06	-10.00	-18.06	FeS2
Melanterite	-4.21	-6.57	-2.36	FeSO4·7H2O
Nesquehonite	-3.05	-8.50	-5.45	MgCO3·3H2O
O2(g)	-69.52	-72.43	-2.91	O2
Pyrite	8.80	-10.00	-18.81	FeS2
Pyrochroite	-10.03	5.17	15.20	Mn(OH)2
Pyrolusite	-29.30	13.96	43.26	MnO2
Rhodochrosite	-1.33	-12.42	-11.09	MnCO3
Schwertmannite(1)	-53.77	-43.27	10.50	Fe8O8(OH)4.4(SO4)1.8:8.4H2O
Schwertmannite(2)	-50.85	-32.85	18.00	Fe8O8(OH)6SO4
Siderite	-0.36	-11.18	-10.82	FeCO3
Sulfur	-1.88	3.28	5.16	S
Troilite	-0.04	-6.17	-6.13	FeS

End of simulation.

Reading input data for simulation 9.

End of run.

Appendix D
EMP Supporting Materials

METHODOLOGY

Overview

Analyses on a single grain of soil or a single crystal of a precipitate were accomplished using an EMP. Not only can analyses be made on particles as small as 1 micron, but the EMP also provides a visual picture of the soil at magnifications ranging from 40 to 300,000 times. The visual mode is referred to as the "backscatter mode." Information about the relative atomic number of the compounds can be obtained in the backscatter mode due to the contrast in brightness between the low atomic number compounds and the compounds with high atomic numbers. For example, arsenic and iron compounds, which have high mean atomic numbers, tend to be bright white in backscatter mode, while silica compounds, with lower mean atomic numbers, are gray and organic carbon is nearly black. Direct visual inspection of the soil also provides information on the associations, morphology, and any reaction rims on the particles, all of which provide insight into the geochemical history of the sample. Soil samples were analyzed on a JEOL 8600 Superprobe located in the Department of Geological Sciences, University of Colorado, Boulder, Colorado.



Sample Preservation and Drying

Samples were received at the University of Colorado Laboratory for Environmental and Geological Sciences (LEGS) on December 27th 2007. The samples arrived frozen under dry ice to minimize potential oxidation of any reduced phases that may have been present. The samples were placed under dry ice at LEGS until the samples could be prepped for mounting. The samples were first dried in a sealed chamber using a stream of nitrogen gas. The chamber was equipped with two barbed hose fittings, one to attach to a tank of nitrogen gas and the other to provide an escape route for the moist nitrogen exiting the chamber. The chamber was maintained under a positive nitrogen pressure until the samples were dry. The dried samples were then transferred to a clove box where the process of preparing the epoxy grain mounts was initiated.

Sample Mount Preparation

A 1 gram split of each nitrogen-dried sample was used to prepare epoxy grain mounts within a glovebox. The procedure for preparing the mounts included pouring the sample into a 1-inch diameter mold and covering with a thin layer of air-cured epoxy. The grains were then blended with the epoxy using a disposable wood stirring rod and additional epoxy was added. After curing at room temperature within the glove box, the mount was removed and ground flat, forming a cross sectional cut through the grains. Polishing of the mount was performed using successively finer grades of oil-based diamond paste. The grinding and polishing steps involved the use of equipment that was too large to fit in the glove box, so these steps were performed under ambient oxygen conditions. The final step in the preparation of the grain mounts was to apply a thin carbon coating to the surface of the mount or "puck" in order to allow proper conduction during microprobe analysis. The pucks were then stored in the glove box until the EMP analyses could be performed.



Operating Conditions

Operating conditions included a 15 KeV accelerating voltage, 17 NanoAmp cup current, and a 1 to 2 micron beam size. Certified pure element standards were used to determine phase compositions. Wavelength dispersive spectrometer (WDS) crystals PET for iron and sulfur and LDE1 for oxygen were used for the WDS analyses.

Analytical Procedure

Sample pucks were scanned for iron-containing minerals using backscattered electron images. The scanning was done manually by systematically traversing from left to right until the edge of the mount was reached. The puck was then moved up one field of view and scanned from right to left. This process was repeated until the whole mount was scanned.

Typically, the magnification used for scanning samples was 40-100X and 300-600X, depending on the individual sample's grain size distribution. The last setting allowed the smallest identifiable (1 to 2 μm) phases to be found. Once a candidate particle was identified, then the backscatter image was optimized to discriminate any different phases within the particle or its association. Identification of the iron-bearing phases was done using both energy-dispersive and wavelength-dispersive spectrometers set for analyses of sulfur, iron, and oxygen. A macro was prepared to take into account the absorption of x-rays by elements such as iron using a Zaph correction.

Samples Analyzed

A total of 32 samples were analyzed by EMP, as shown in **Table 1** below.

Table 1 - Summary of Samples Analyzed by Electron Microprobe (EMP)

Sample ID	Description
EPA-C1-A	Altus Air Force Base
EPA-C3-A	Altus Air Force Base
EPA-C4-A	Altus Air Force Base
EPA-C5-A	Altus Air Force Base
EPA-C6-A	Altus Air Force Base
EPA-C7-A	Altus Air Force Base
EPA-C11-A	Altus Air Force Base
EPA-C13-A	Altus Air Force Base
EPA-C15-A	Altus Air Force Base
B3 1-1	Mulch Biowall Column Experiment, Slice 1, Section 1
B3 3-1	Mulch Biowall Column Experiment, Slice 3, Section 1
B3 5-1	Mulch Biowall Column Experiment, Slice 5, Section 1
B3 7-1	Mulch Biowall Column Experiment, Slice 7, Section 1
DTSB-1-10	Dover Air Force Base
DTSB-1-17	Dover Air Force Base
DTSB-3-10	Dover Air Force Base
DTSB-3-16	Dover Air Force Base
DTSB-6-10	Dover Air Force Base
DTSB-8-10	Dover Air Force Base
DTSB-8-17	Dover Air Force Base
UTSB-16-10	Dover Air Force Base
SA1-9-11	Seneca Air Force Base
SA1-6-8	Seneca Air Force Base
SB1-7-9	Seneca Air Force Base
SB1-7.5-9.5	Seneca Air Force Base
97S-0086	Dugway Air Force Base
97S-0087	Dugway Air Force Base
97S-0088	Dugway Air Force Base
97S-0089	Dugway Air Force Base
97S-0090	Dugway Air Force Base
97FD-0090	Dugway Air Force Base
97S-0091	Dugway Air Force Base

RESULTS

The iron phases in the samples were identified by the backscatter images and by using the Zaph-corrected compositions as compared to the composition of various pure phases. Tables 1 and 2 show the compositions of the iron sulfides and iron oxide/hydroxides, respectively.

Table 1 – Iron Sulfide Minerals and the Stoichiometric Compositions.

Phase	Formula	Composition
Iron Monosulfide	FeS	63.5% Fe, 36.5% S
Pyrrhotite	Fe _{1-x} S	59.1-63.5% Fe, 36.5-40.9% S
Greigite	Fe ⁺² Fe ⁺³ ₂ S ₄	56.6% Fe, 43.4% S
Pyrite/Marcasite	FeS ₂	46.6% Fe, 53.4% S

Table 2 – Iron Oxide/Hydroxide Minerals and the Stoichiometric Compositions.

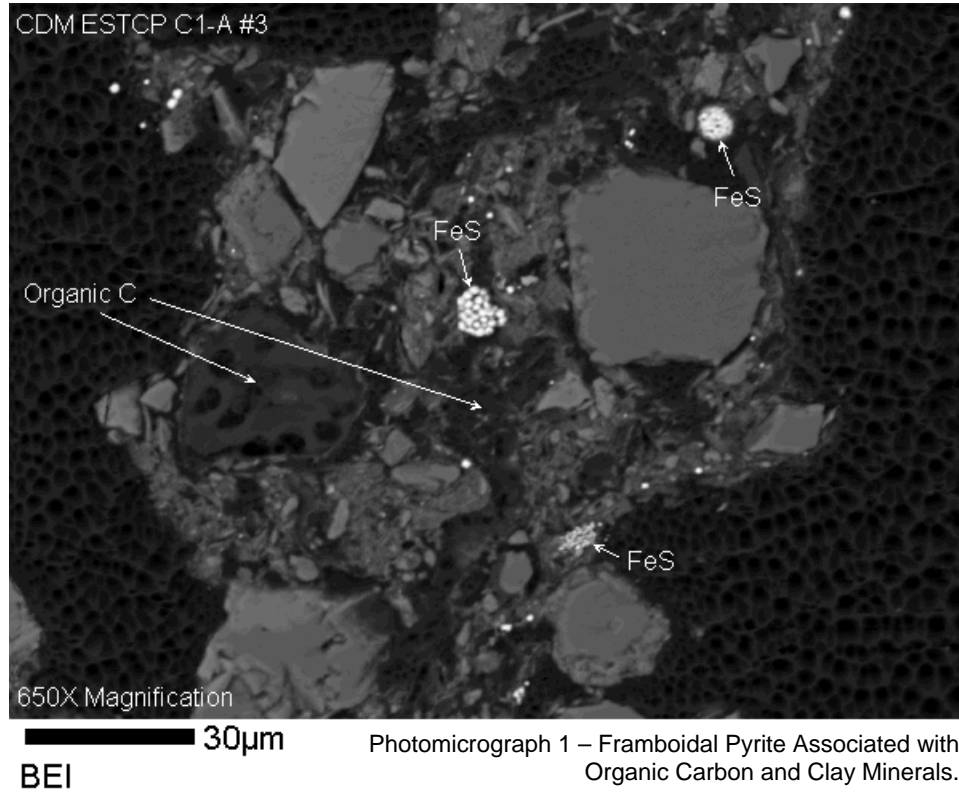
Phase	Formula	Composition
Ferric Hydroxide	FeOOH	62.9% Fe, 36.0% O, 1.1% H
Hydrated Ferric Hydroxide	FeOOH · nH ₂ O	<62.9% Fe (composition depends on value of n)
Magnetite	Fe ₃ O ₄	72.4% Fe, 27.6% O
Hematite	Fe ₂ O ₃	69.9% Fe, 30.1% O
Ferrous Hydroxide	Fe(OH) ₂	62.2% Fe, 35.6% O, 2.2% H
Sulfate Green Rust	[Fe ⁺² ₄ Fe ⁺³ ₂ (OH) ₁₂] ²⁺ · [SO ₄ · nH ₂ O] ²⁻	<53.8% Fe, <5.1% S, >41.1% O (composition depends on value of n)
Hydroxy Green Rust	[Fe ⁺³ _(1-x) Fe ⁺² _x (OH) ₂] ^{x+} · [xOH ⁻ · nH ₂ O] ^{x-}	<62.2% Fe, >35.6% O (composition depends on value of n)

The analysis macro reported both the raw percentages, as well as the compositions when normalized to 100%. In some cases, such as when other elements were likely present that were not analyzed, the raw values were more useful. In other cases, such as when very small grains were analyzed (and the electron beam was focused partly on the epoxy grain mount during the analysis) the normalized values were more appropriate.

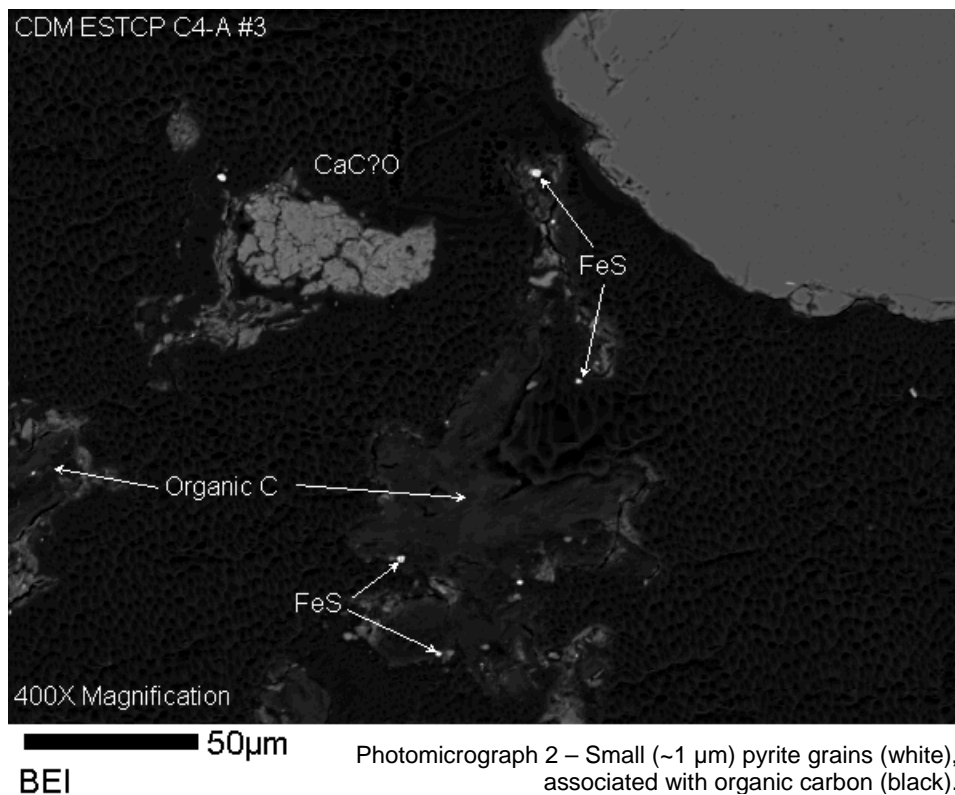
Altus Air Force Base

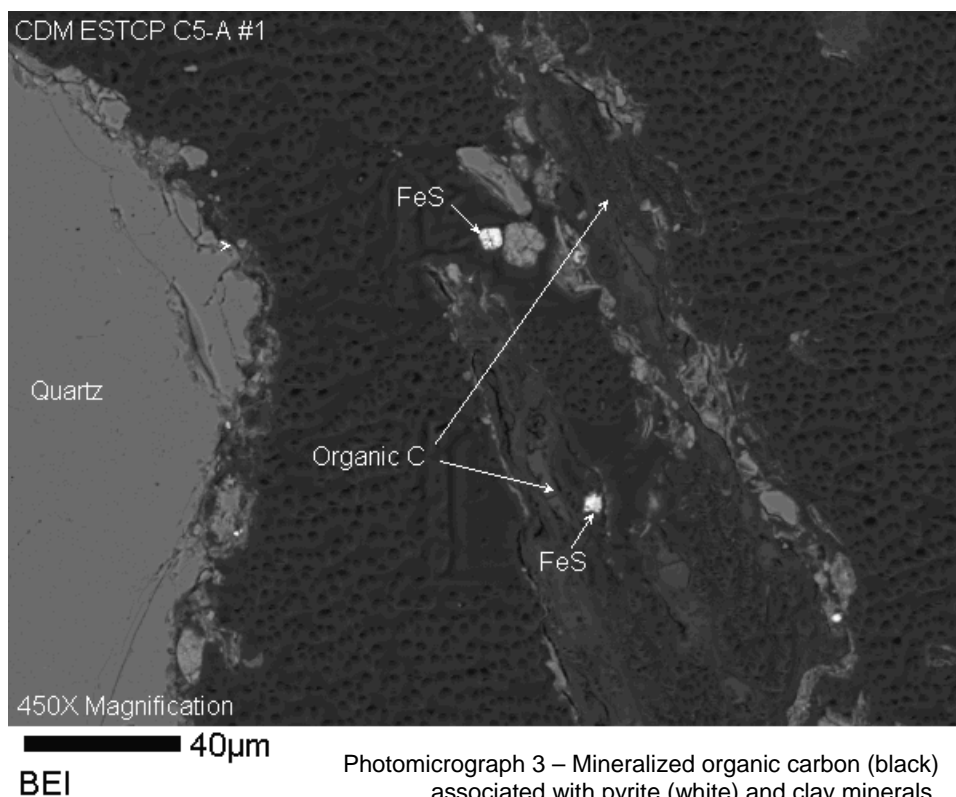
The Altus AFB biowall samples contained quartz, clay minerals, organic matter, and an iron sulfide mineral consistent with pyrite (see attachment 1 for analyses).

Photomicrograph 1 illustrates each of the phases found in the samples. The pyrite was present in two forms, framboidal and granular. In general, the granular forms were small (~1 µm) and were often directly associated with organic matter. The framboidal forms appeared larger, but on close inspection are composed of aggregates of 1 µm particles (Photomicrograph 1).



An example of the granular form, illustrating the association with organic carbon is shown in Photomicrograph 2. Also shown is a mineral containing calcium and oxygen, which is likely calcium carbonate (the EMP can not quantify carbon).





Photomicrograph 3 shows granular pyrite grains associated with “mineralized” organic carbon. Mineralized organic matter had both the characteristic broad “hump” associated with organic matter as well as some well defined peaks (see Figure 1). The minerals apatite ($\text{Ca}_5(\text{PO}_4)_3(\text{F}, \text{Cl}, \text{OH})$) and pyrite appear to have precipitated within the open spaces between the cell walls.

Another form of reduced iron besides pyrite was identified in the samples; magnetite (Fe_3O_4). The identification was made using the stoichiometry of the mineral compared to the measured iron and oxygen contents (see Attachment 1 and Table 2). An example of a magnetite grain is shown in Photomicrograph 4.

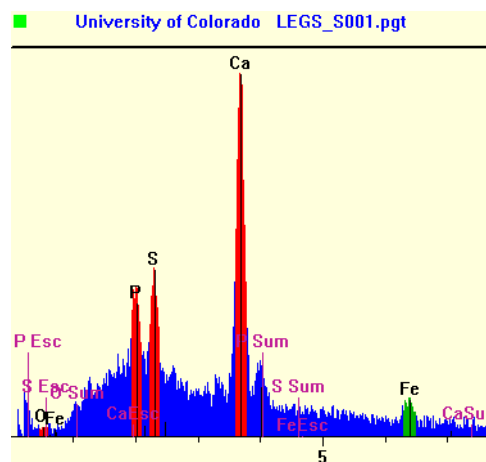
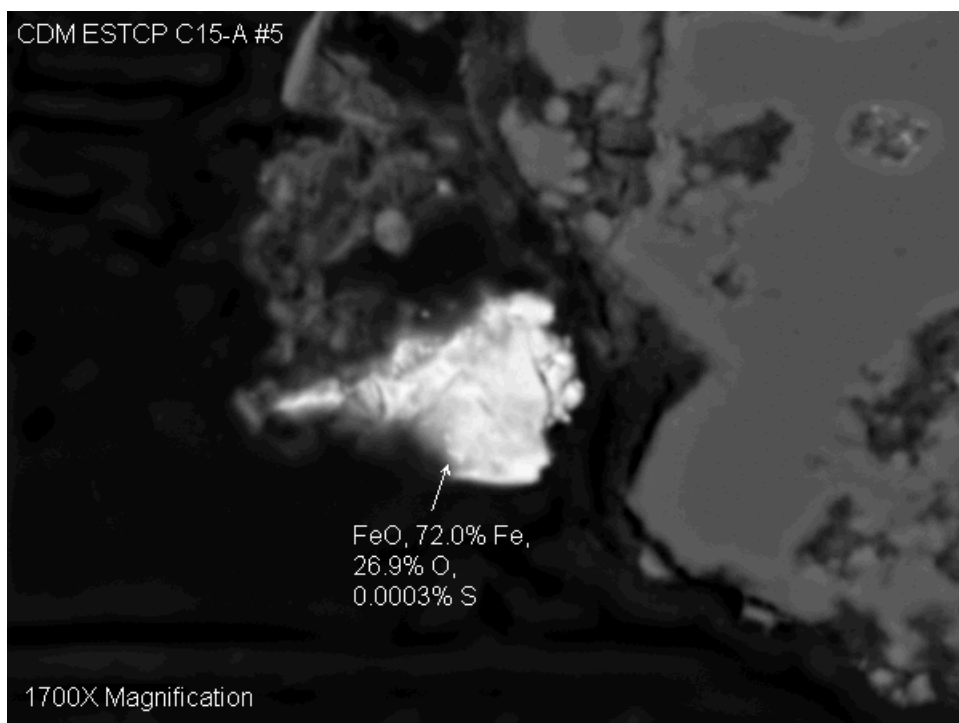


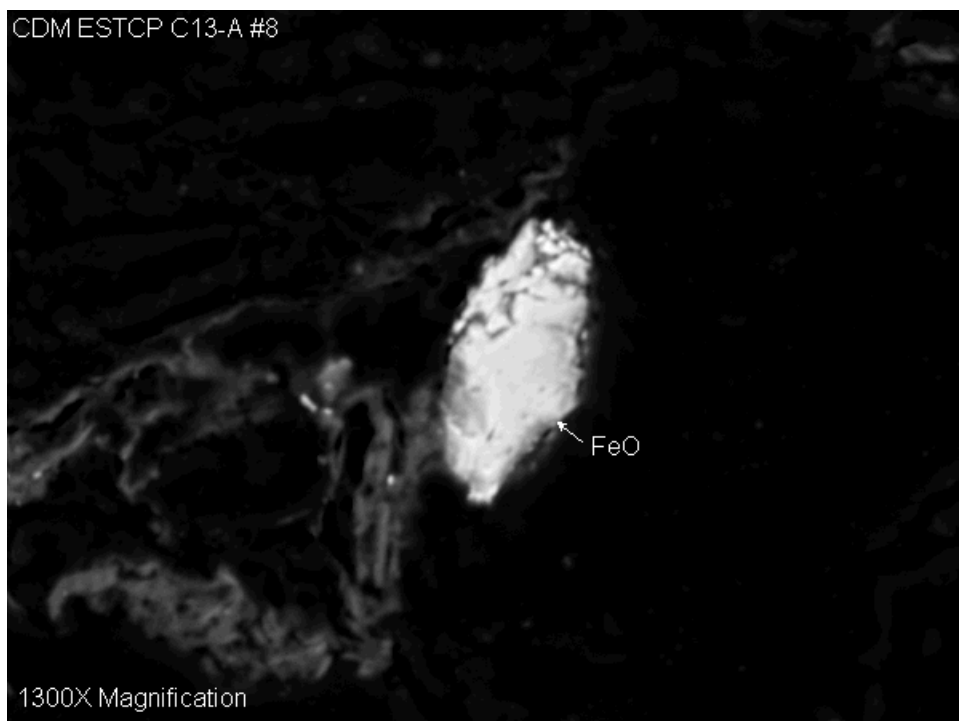
Figure 1 – EDXRF Spectra of mineralized organic carbon.



10µm
BEI

Photomicrograph 4 – Iron oxide mineral consistent with the mineral magnetite. The phase appears to be secondary.

The grain does not have the even, consistent tone seen on backscatter images of crystalline primary minerals, but instead shows a mottled combination of white and gray areas across the grain, suggesting a secondary origin. Another example of the magnetite found in the sample is shown in Photomicrograph 5.



10µm
BEI

Photomicrograph 5 – Grain of magnetite, possibly of secondary origin.

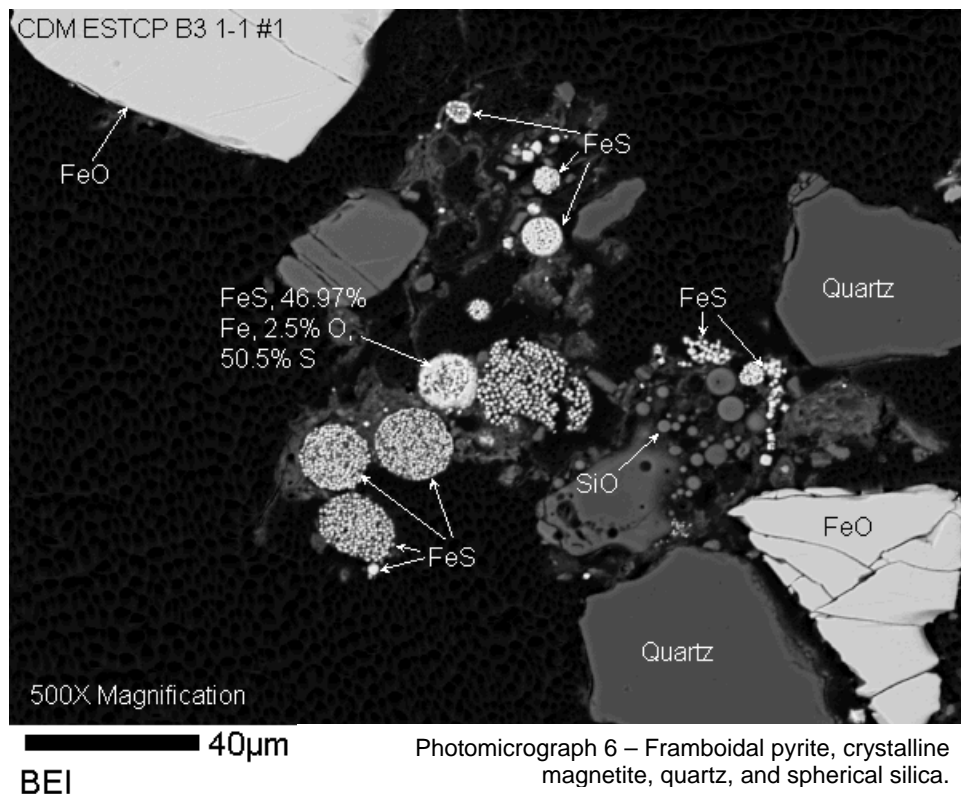
As a general rule, samples C1-A through C6-A were characterized by pyrite, and samples C11-A, C13-A, and C15-A were characterized by magnetite, while sample C7-A contained both phases, as shown in the summary in **Table 3**.

Table 3 - Summary of Reduced Iron Phases in Altus AFB Samples Analyzed by Electron Microprobe (EMP)

Sample ID	Phases and Associations
EPA-C1-A	Granular and Framboidal Pyrite (FeS_2)
EPA-C3-A	Granular Pyrite (FeS_2), typically 1 μm diameter in assoc. with organic carbon and clay minerals.
EPA-C4-A	Granular Pyrite (FeS_2), typically 1 μm diameter in assoc. with organic carbon and clay minerals. Also Framboidal Pyrite.
EPA-C5-A	Granular Pyrite (FeS_2), typically 1 μm diameter in assoc. with organic carbon and clay minerals.
EPA-C6-A	Granular and Framboidal Pyrite (FeS_2) usually associated with organic carbon.
EPA-C7-A	Granular and Framboidal Pyrite (FeS_2) and Crystalline Magnetite (Fe_3O_4)
EPA-C11-A	Crystalline Magnetite (Fe_3O_4)
EPA-C13-A	Crystalline Magnetite (Fe_3O_4)
EPA-C15-A	Crystalline and Secondary Magnetite (Fe_3O_4) and one grain of Iron Metal

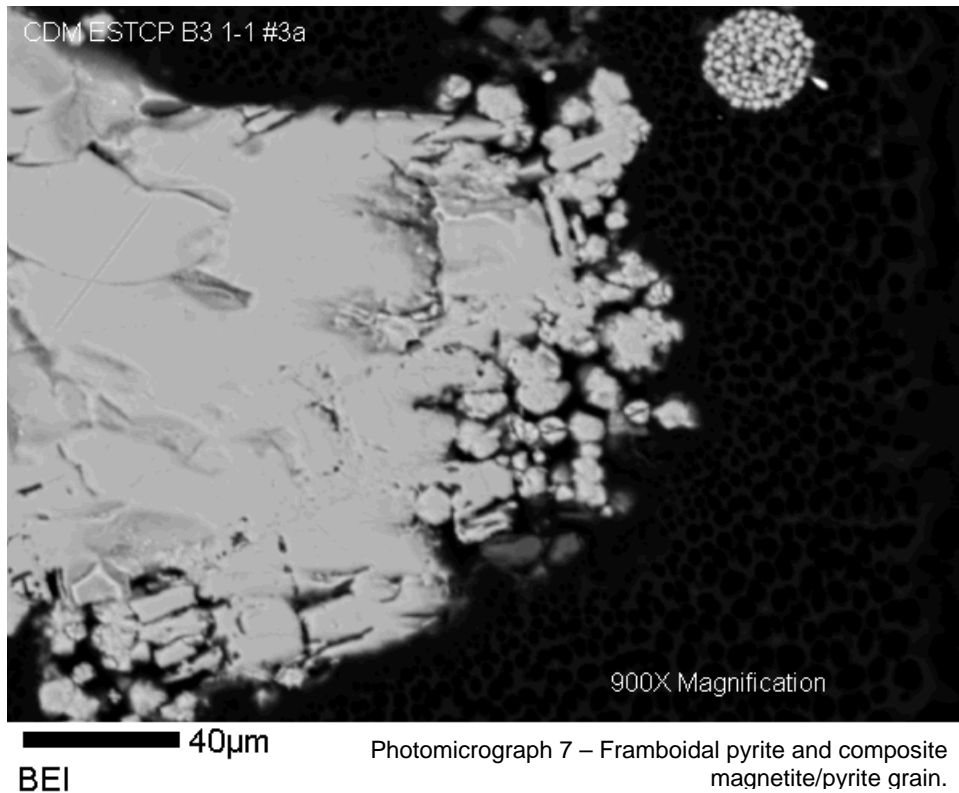
EPA Column Samples

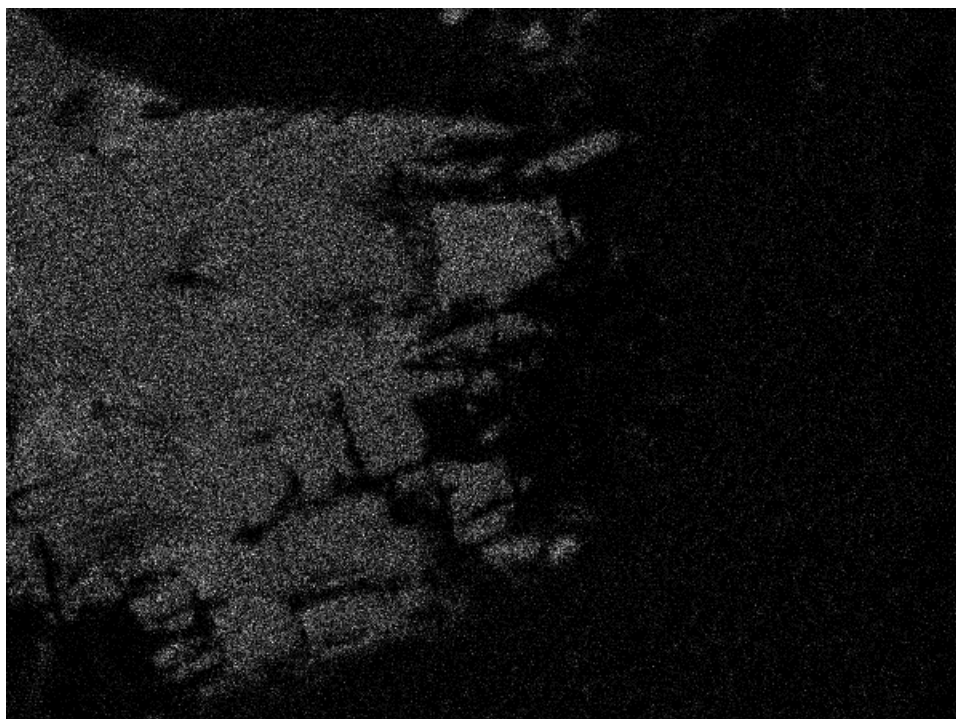
The column samples were characterized by pyrite, quartz, crystalline magnetite, organic carbon, and a phase that may be green rust or partially oxidized pyrite. Another interesting phase was a spherical form of silica (see Photomicrograph 6).



Photomicrograph 6 – Framboidal pyrite, crystalline magnetite, quartz, and spherical silica.

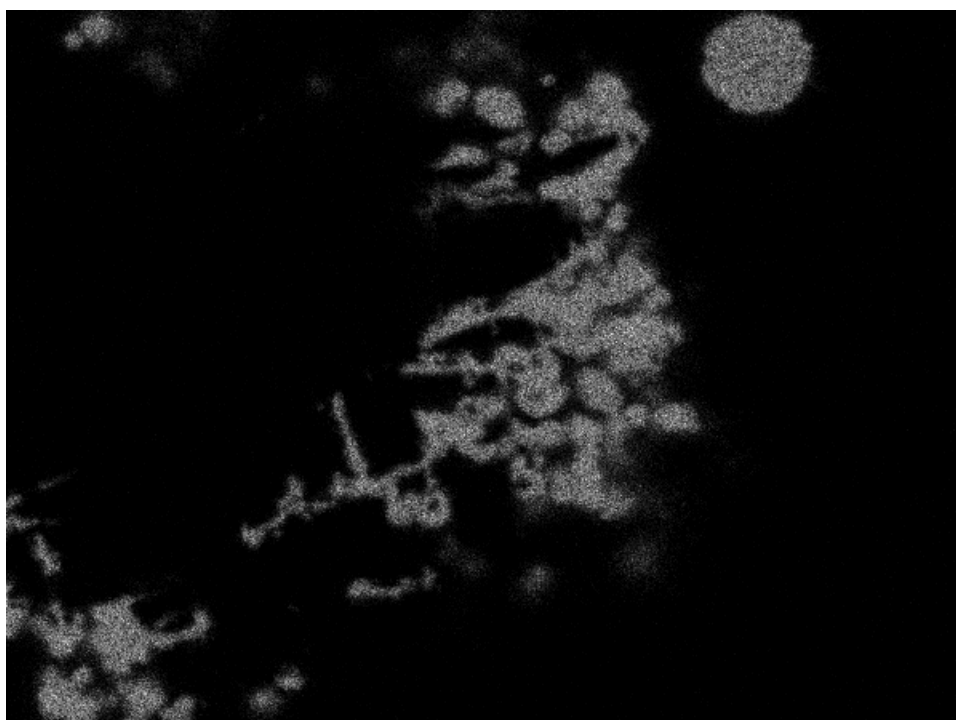
The magnetite shown in photomicrograph 6, unlike those in photomicrographs 4 and 5, has a very even tone across the grains, suggesting that they are crystalline. The framboidal forms of pyrite were abundant in the samples. Pyrite also occurred in a more granular form, which was often associated with crystalline magnetite, even to the point of coating the grains and filling in voids and fractures. Photomicrograph 7 shows a grain containing both pyrite and magnetite. The pyrite is difficult to distinguish from the magnetite in photomicrograph 7 due to the similar degree of backscattering. Therefore, in order to illustrate the two phases, element maps or “dot maps” were prepared (see Photomicrographs 8 and 9). Photomicrograph 8 shows the distribution of oxygen across the grain. Note that the higher densities of white dots correspond with higher concentrations of oxygen within the phase. By comparing Photomicrographs 7 and 8, it is clear that what appears to be a homogenous mineral in photomicrograph 7 is actually composed of two very closely associated phases, one with a significant content of oxygen, and the other with little or no oxygen. WDS analyses of each phase indicate the presence of both magnetite and pyrite.





40μm
O

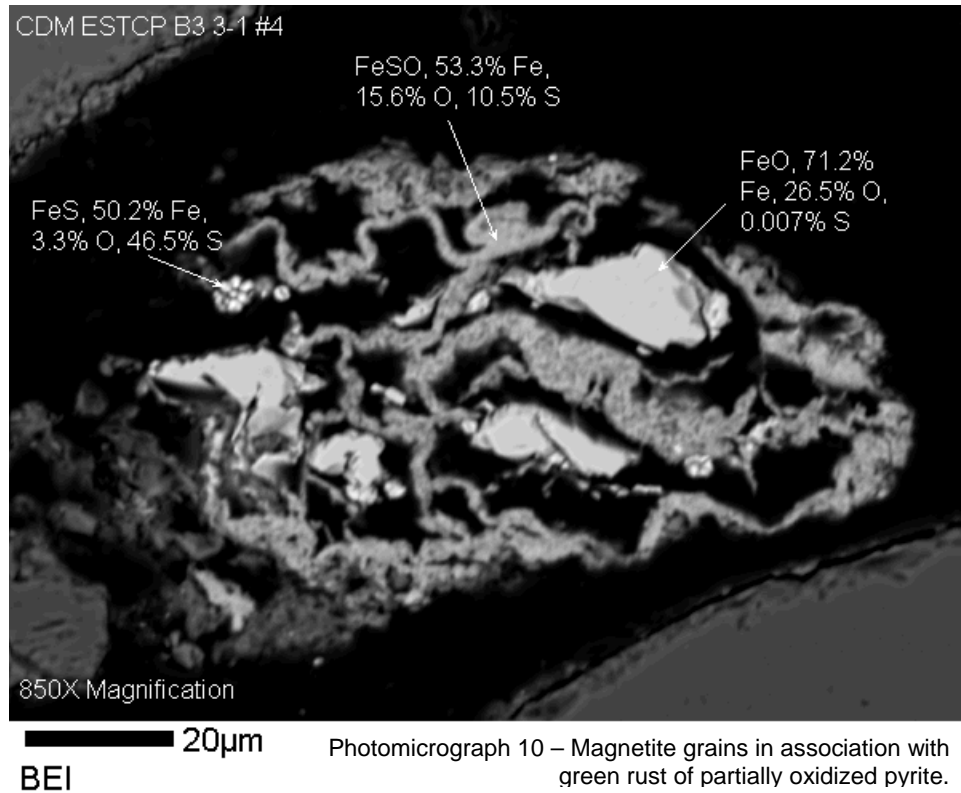
Photomicrograph 8 – Element map showing the distribution of oxygen across the grain.



40μm
S

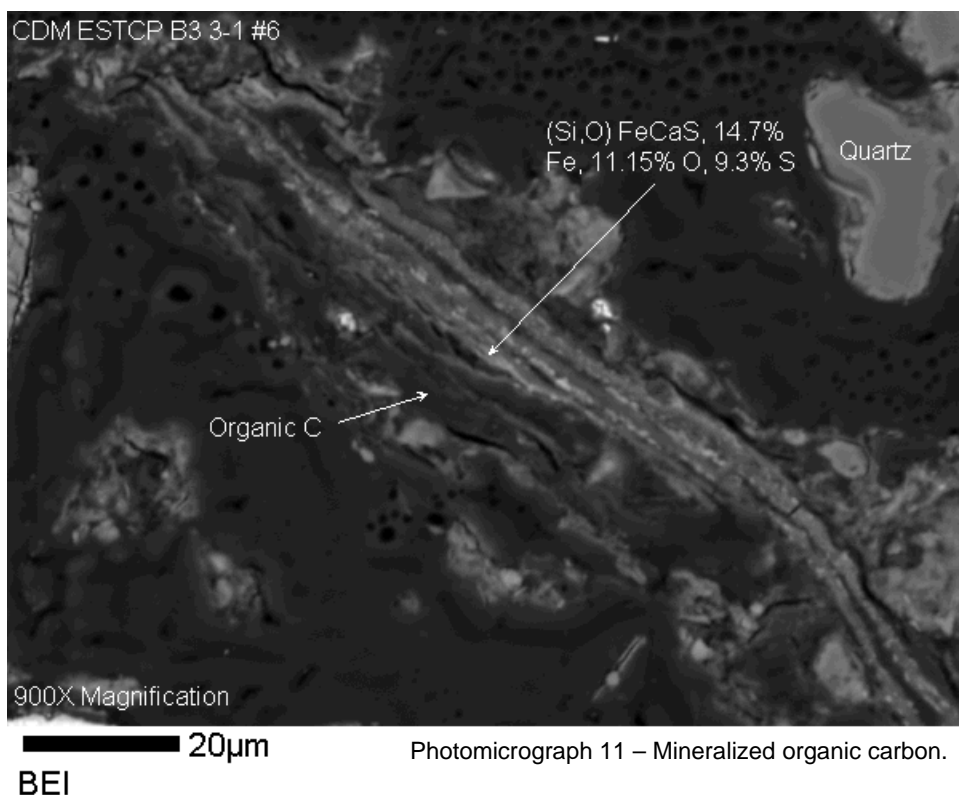
Photomicrograph 9 – Element map showing the distribution of sulfur across the grain.

Photomicrograph 9 shows the element map for sulfur, which clearly illustrates the areas where pyrite is present. The element maps help to illustrate the intimate association of pyrite and magnetite, including filling of voids and fractures in the magnetite with pyrite.



An apparently secondary phase which may be green rust was found in two of the samples is shown in Photomicrograph 10. The phase had about 55% iron, 20% oxygen, 7% sulfur, and the balance unanalyzed. The phase does not appear to be jarosite ($\text{HFe}_3(\text{SO}_4)_2(\text{OH})_6$), which has much more oxygen (48%) and less iron (36%).

Like the Altus samples, the EPA column samples also contained mineralized organic carbon, as shown in Photomicrograph 11.



A summary of the phases identified within each slice of the column is provided in **Table 4**.

Table 4 – Summary of Reduced Iron Phases in EPA Column Samples Analyzed by Electron Microprobe (EMP)

Sample ID	Phases and Associations
B3 1-1	Granular Pyrite often Associated with Magnetite (Fe_3O_4). Framboidal Pyrite often associated with Organic Carbon. Spherical silica also noted.
B3 3-1	Pyrite associated with magnetite and Organic Carbon. Partially oxidized pyrite and/or green rust.
B3 5-1	Granular Pyrite often Associated with Magnetite (Fe_3O_4). Framboidal Pyrite often associated with Organic Carbon.
B3 7-1	Pyrite associated with magnetite, hematite, and Organic Carbon. Partially oxidized pyrite and/or green rust.

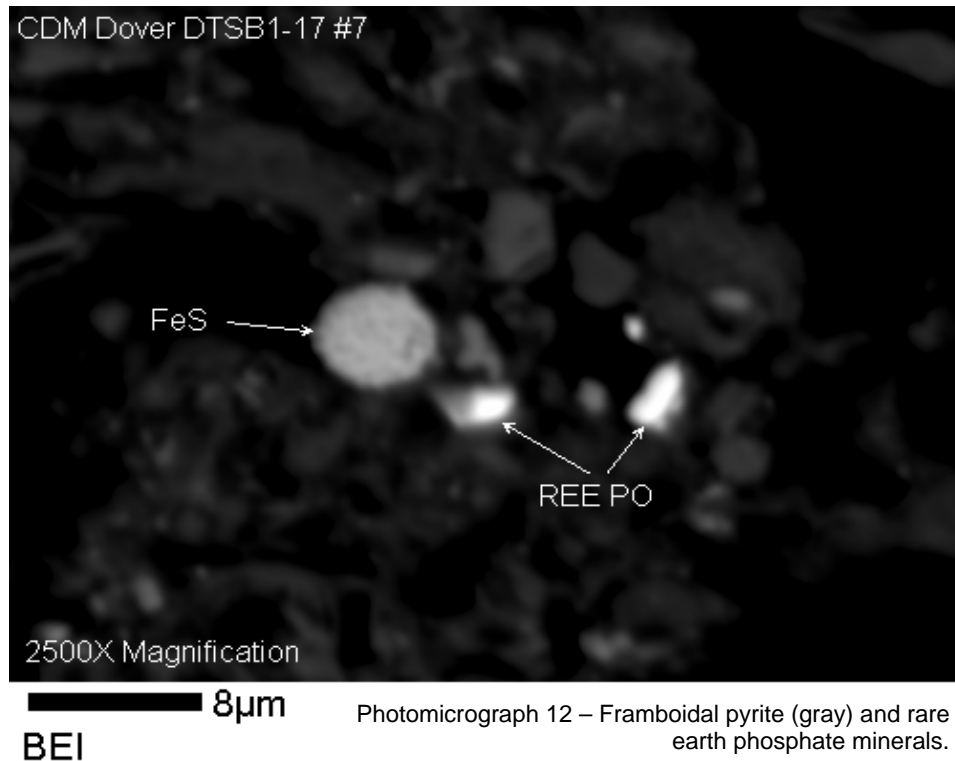
No clear trends were identified within the length of the column.

Dover Air Force Base

The reduced iron phases identified in the Dover samples included, partially oxidized pyrite and iron monosulfides, ferrous iron oxides or hydroxides some consistent with green rust, and iron silicate. Ferrous iron was also present within ilmenite (FeTiO_3),

which is likely a primary mineral. Another reduced phase was native copper, which when found, was generally small and associated with organic carbon.

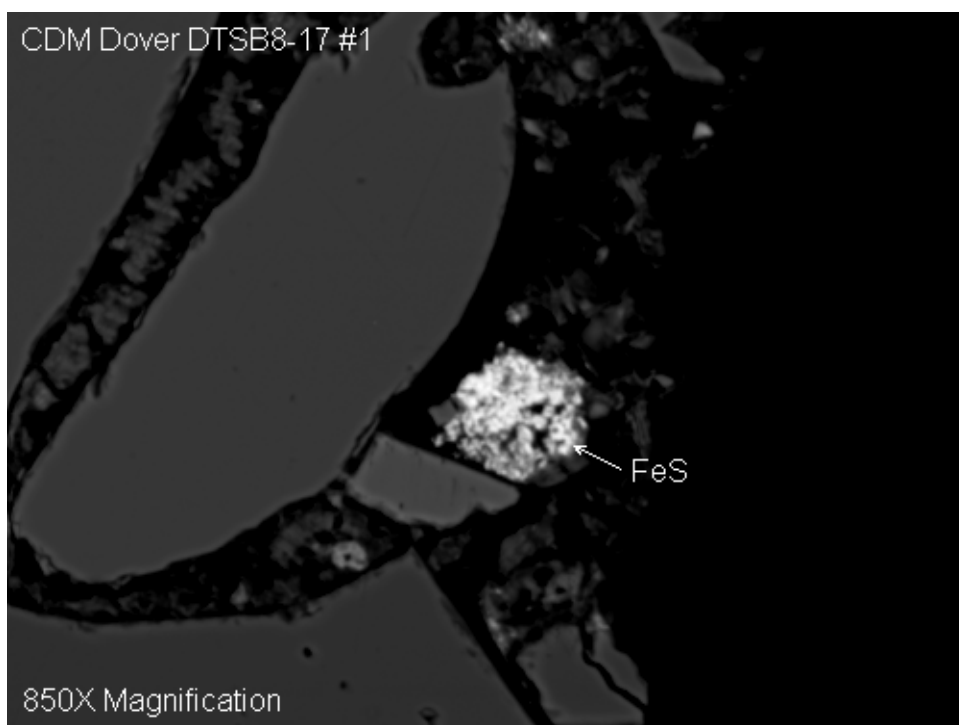
Partially oxidized iron sulfides were the most abundant reduced iron phases. Photomicrograph 12 shows an example of an iron sulfide mineral with a framboidal form which contained 49.8% iron, 2.8% oxygen, and 47.3% sulfur (normalized).



The composition corresponds to a formula of $\text{FeS}_{1.8}\text{O}_{0.2}$, which is consistent with partially oxidized pyrite. The brighter grains shown in Photomicrograph 12 are rare earth phosphate minerals, which are commonly found in soils.

An example of an iron sulfide mineral which appears to be consistent with partially oxidized iron monosulfide is shown in Photomicrograph 13. The normalized composition was 62.2% iron, 5.4% oxygen, and 32.3% sulfur, which corresponds to a formula of $\text{FeS}_{0.9}\text{O}_{0.3}$.

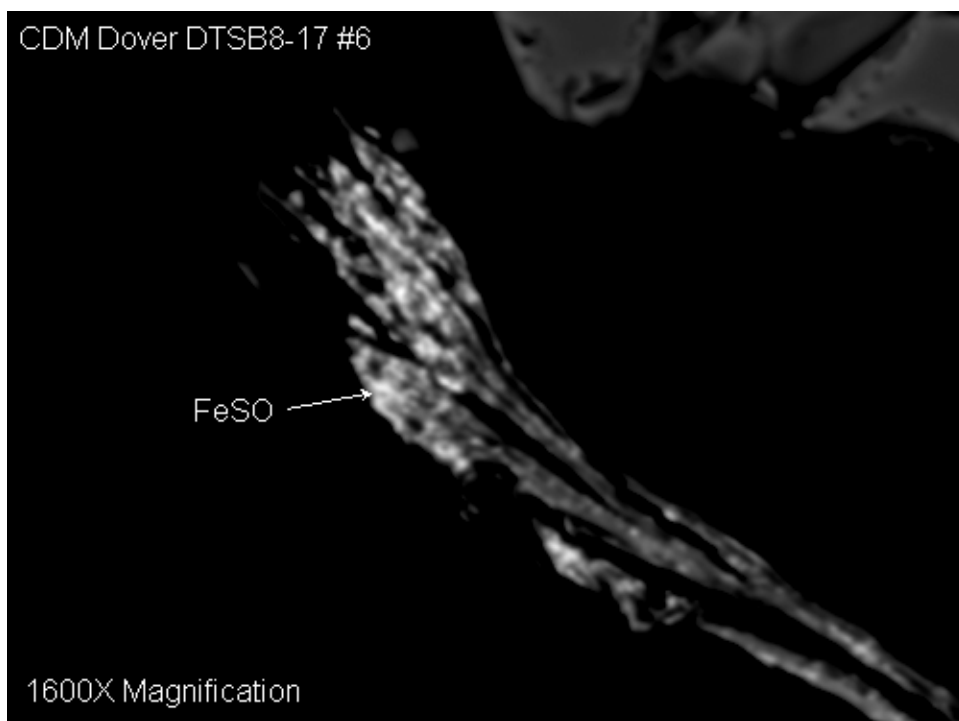
An example of a completely oxidized iron monosulfide in association with a platy silicate mineral such as clay or mica, is shown in Photomicrograph 13. The normalized composition of the iron sulfide phase was 56.6% iron, 16.4% oxygen, and 26.9% sulfur, corresponding to a formula of $\text{FeS}_{0.8}\text{O}_{1.0}$, which is essentially ferrous sulfate.



20µm

BEI

Photomicrograph 13 – Partially oxidized iron monosulfide.

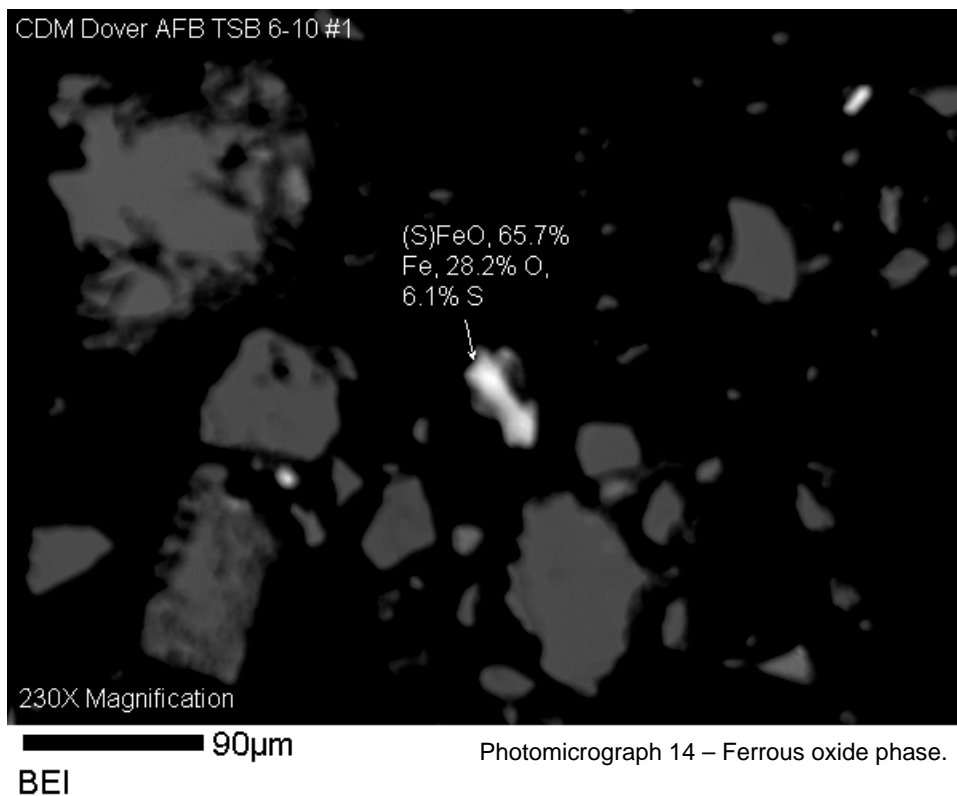


10µm

BEI

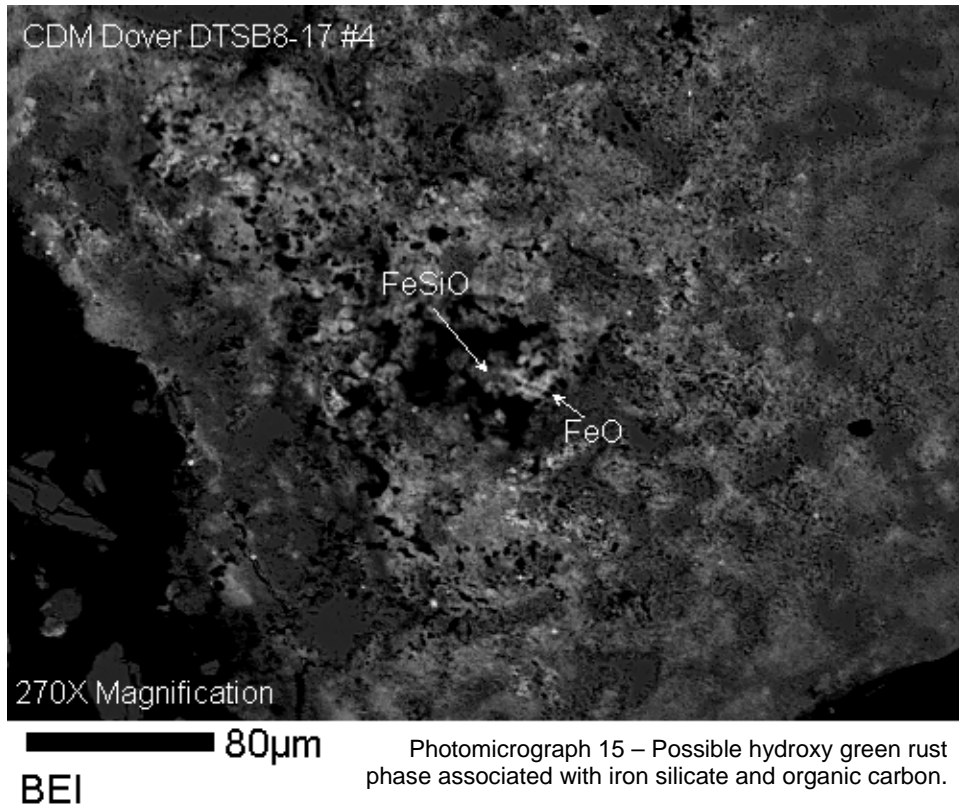
Photomicrograph 14 – Oxidized iron monosulfide associated with a platy silicate mineral (clay or mica).

Grains consistent with the composition of green rust were also found in the sample. Photomicrograph 14 is an example of a potential green rust phase, with the normalized composition of 65.7% iron, 28.2% oxygen, and 6.0% sulfur.

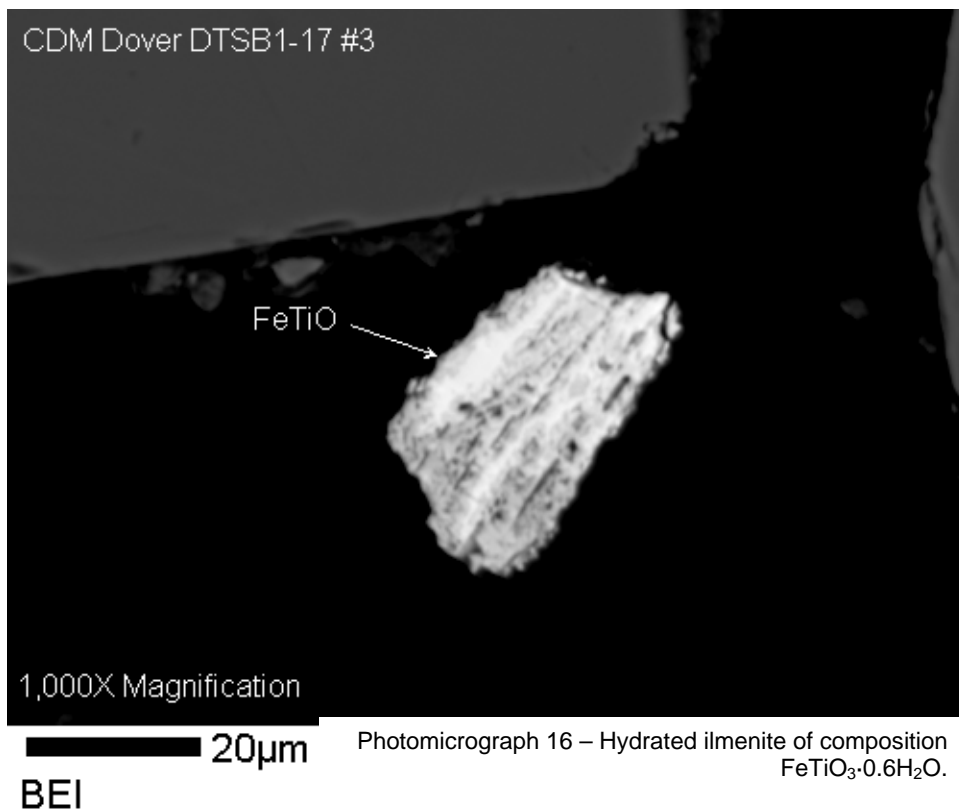


Genin 2001 gives the formula $[\text{Fe}^{\text{II}}_4\text{Fe}^{\text{III}}_2(\text{OH})_{12}]^{2+} \cdot [\text{SO}_4 \cdot n\text{H}_2\text{O}]^{2-}$ for sulfate green rust, which has a molar Fe:S ratio of 6:1. The Fe:O ratio varies depending on the number of water molecules (n) in the formula, but it must be less than 0.38:1 (assumes $n=0$). The phase in question has an Fe:S ratio of 6.25:1, but the Fe:O ratio is 0.67:1, which is too high for green rust (not enough oxygen). The phase would have the formula $\text{Fe}(\text{SO}_4)_{0.16}\text{O}_{0.85}$, which is a ferrous oxide with substituted sulfate.

Another potential green rust phase is shown in Photomicrograph 15 from sample DTSB-8-17. The phase had 46.3% iron and 52.0% oxygen. The formula depends on the assumed oxidation state of iron and on the degree of hydration. Assuming all of the iron is ferric, the formula would be $\text{Fe}(\text{OH})_3 \cdot 0.9\text{H}_2\text{O}$, while for ferrous iron it would be $\text{Fe}(\text{OH})_2 \cdot 1.9\text{H}_2\text{O}$. Green rusts are a mixture of ferrous and ferric iron. Hydroxy green rust has the general formula $[\text{Fe}^{\text{II}}_{(1-x)}\text{Fe}^{\text{III}}_x(\text{OH})_2]^{x+} \cdot [x\text{OH}^- \cdot n\text{H}_2\text{O}]^{x-}$ and contains a minimum of 35.6% oxygen (when $x=0$ and $n=0$). Additional oxygen is added as ferric iron is added (x increases) and/or water is added (n increases). However, without knowing the amount of hydrogen in the phase it is not possible to determine the stoichiometry.



Another form of ferrous iron which was identified in the samples was a phase that compositionally resembles the primary mineral ilmenite (FeTiO_3), but tends to have more oxygen and has a definite secondary or weathered appearance. An example is shown in Photomicrograph 16.



A summary of the ferrous iron phases for each of the Dover AFB samples is presented in Table 5.

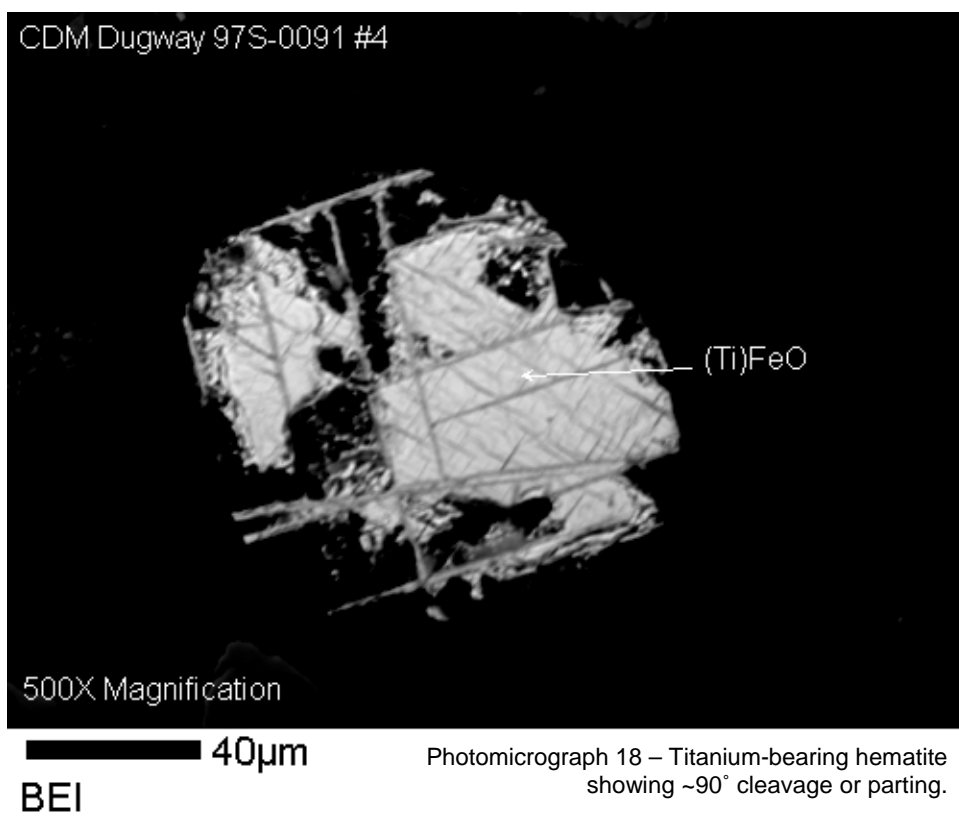
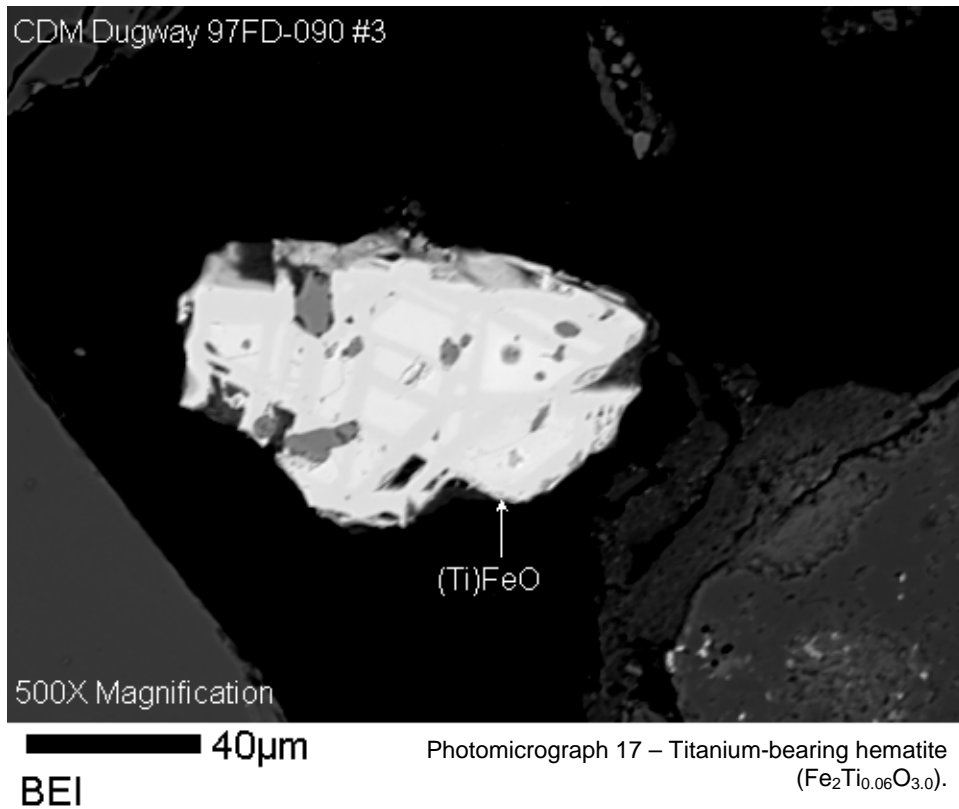
Table 5 - Summary of Reduced Iron Phases in the Dover AFB Samples Analyzed by Electron Microprobe (EMP)

Sample ID	Phases and Associations
DTSB-1-10	Partially to completely oxidized pyrite, iron silicate, and possible magnetite and green rust.
DTSB-1-17	Partially oxidized iron sulfides (iron monosulfides and pyrite), hydrated ilmenite, ferrous oxide and hydroxide and possible green rust.
DTSB-3-10	Partially oxidized iron sulfides (iron monosulfides and pyrite) titanium-bearing ferrous iron oxyhydroxide, and iron silicate.
DTSB-3-16*	Partially to completely oxidized iron sulfides (iron monosulfides and pyrite). Possible hydrous ferrous hydroxide, ilmenite, iron-silicon sulfate. (also native copper)
DTSB-6-10	Partially to completely oxidized iron sulfides (iron monosulfides and pyrite) and ferrous oxysulfate.
DTSB-8-10	Partially to completely oxidized iron sulfides (iron monosulfides and pyrite)
DTSB-8-17	Partially to completely oxidized iron monosulfides and possible hydroxyl green rust (only 1 grain).
UTSB-16-10*	Partially to completely oxidized pyrite and hydrous or partially oxidized ilmenite (also native copper)
*Iron analyses were unusually low for samples DTSB-3-16 and UTSB-16-10. The instrument was repeaked for iron in the middle of the analysis of sample DTSB-3-16 and the iron results were more reasonable.	

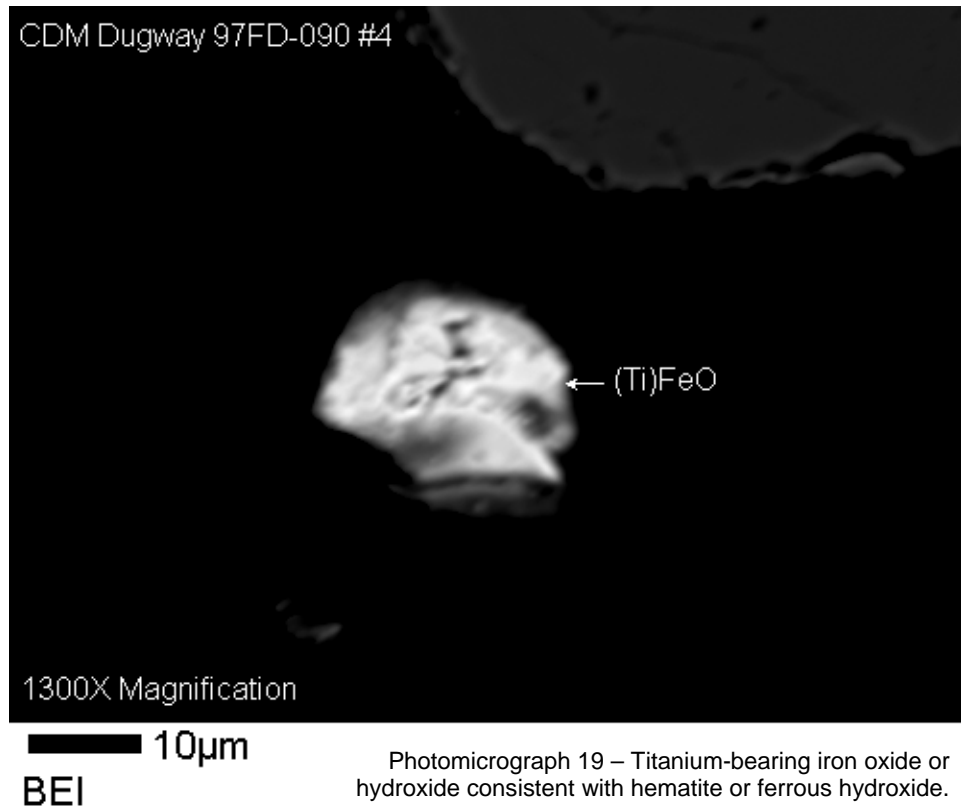
Dugway Proving Ground

The vast majority of the potential ferrous iron phases in the dugway samples consisted of hydrous titanium-bearing iron hydroxides. However, compositionally, these phases were also very close to hematite and in some cases the phase is a clear alteration product of a primary iron mineral. An example is shown in Photomicrograph 17. The phase appears to be crystalline and to be a weathering product of a primary mineral, both of which suggest that the phase is hematite. The phase is composed of 68.7% iron, 29.4% oxygen, and 1.9% titanium, with a composition of $(\text{Fe}_2\text{Ti}_{0.06}\text{O}_{3.0})$. Such a phase could be formed by the weathering and oxidation of titanomagnetite.

Another example of a likely hematite phase is shown in Photomicrograph 18. The phase has the composition; 68.0% Fe, 30.0% O, and 2.0% Ti, with a composition of $\text{Fe}_2\text{Ti}_{0.06}\text{O}_{3.1}$. Parting or cleavage at approximately 90° angles can be seen, which is consistent with the partings of hematite.



However, other examples have a more secondary morphology and the identification is not as clear. An example is shown in Photomicrograph 19.



The phase appears to be porous and to have a variable composition within the grain. The analysis showed that the grain in that location had a composition (normalized) of 58.5% Fe, 33.6% O, and 7.9% Ti. The formula of the phase ($\text{FeTi}_{0.2}(\text{OH})_{2.0}$) is more consistent with a ferrous hydroxide than for hematite. Note that the titanium throws off the charge balance, such that the true formula would be closer to $\text{Fe}^{2+}\text{Ti}_{0.2}\text{O}_2\text{H}_{1.2}$. Another possibility is that the phase contains some ferric iron (instead of some of the hydrogen), for example $\text{Fe}^{3+}\text{Ti}_{0.2}\text{O}_2\text{H}_{0.2}$. The true phase could also contain a mixture of ferrous and ferric iron. The phase highlights the limitations of the EMP technique for identifying iron phases (due to the inability to analyze hydrogen).

Other reduced phases identified in the sample included just a few grains of partially oxidized zinc and lead sulfides (1 grain each) and possible green rust (2 grains).

A summary of the phases found in the Dugway samples is provided in Table 6.

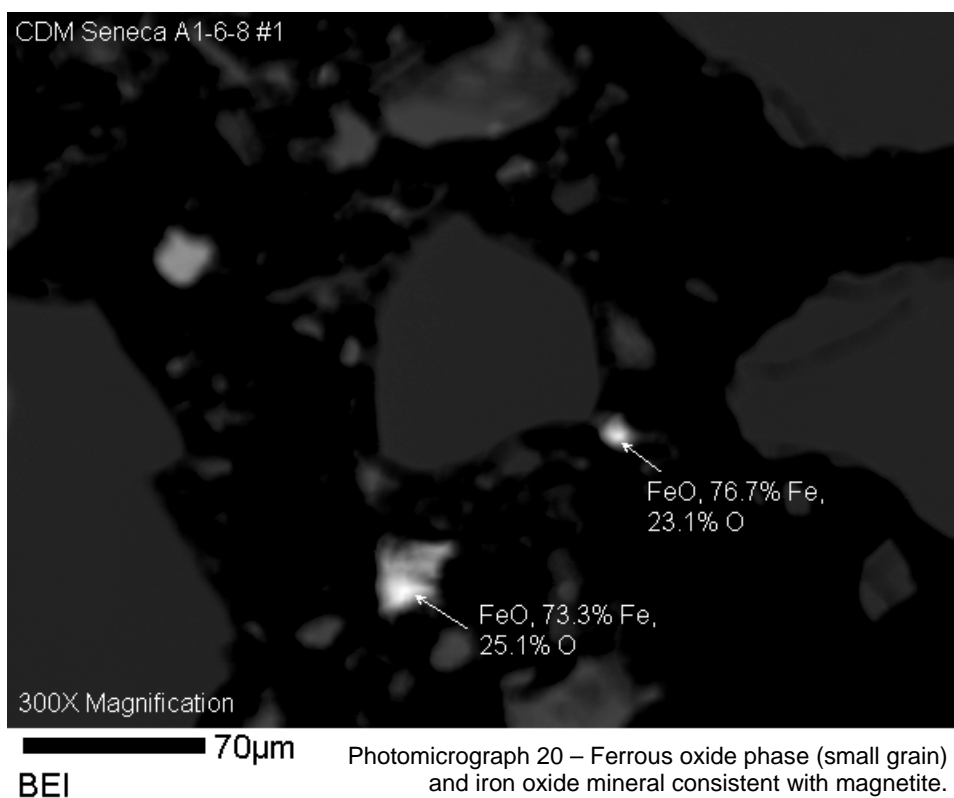
Table 6 - Summary of Reduced Iron Phases in the Dugway Proving Ground Samples Analyzed by Electron Microprobe (EMP)

Sample ID	Phases and Associations
97S-0086	Titanium-bearing hematite and/or titaniferrous hydroxide and partially oxidized zinc sulfide (1 grain)
97S-0087	Titanium-bearing hematite and/or titaniferrous hydroxide

	and potential hydroxyl green rust (2 grains)
97S-0088	Titanium-bearing hematite and/or titaniferrous hydroxide
97S-0089	Titanium-bearing hematite and/or titaniferrous hydroxide and partially oxidized or hydrated ilmenite.
97S-0090	Titanium-bearing hematite and/or titaniferrous hydroxide and lead-bearing iron oxyhydroxysulfate (1 grain)
97FD-0090	Titanium-bearing hematite and/or titaniferrous hydroxide and partially oxidized lead sulfide (1 grain)
97S-0091	Titanium-bearing hematite and/or titaniferrous hydroxide and magnetite (1 grain)

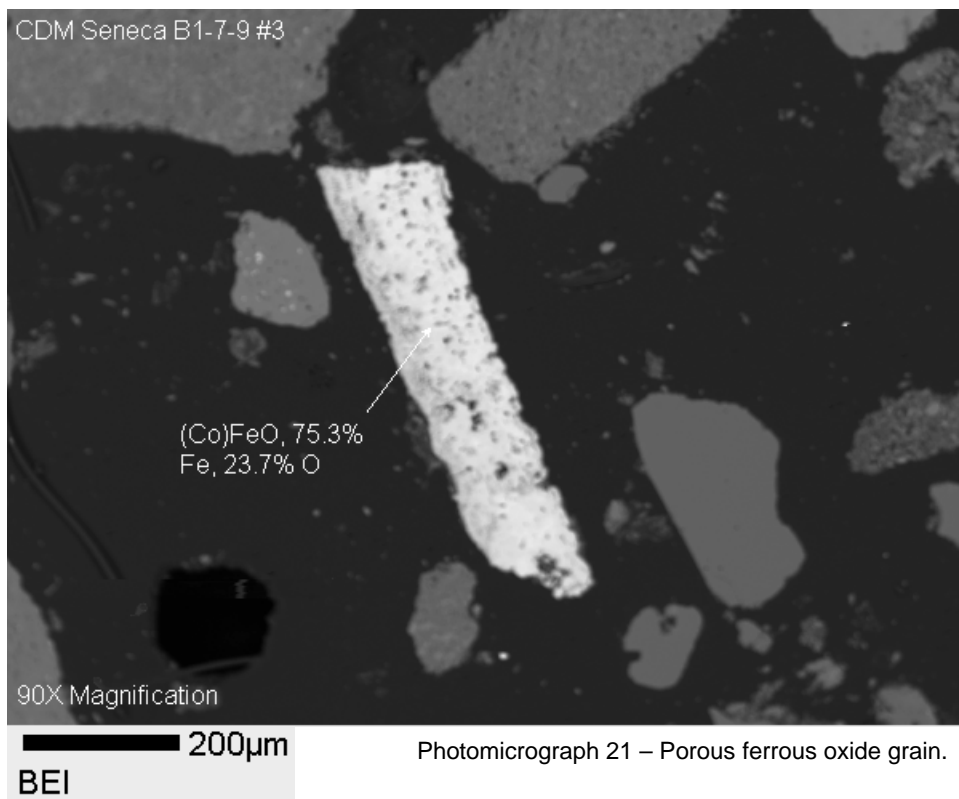
Seneca AFB

The reduced iron phases in the Seneca samples consisted of magnetite, titanium-bearing ferrous oxides, ilmenite, and potentially ferrous hydroxide (could be hematite). An example of probable magnetite and ferrous oxide grains are shown in Photomicrograph 20.



The larger ~30 µm grain has the normalized composition of 73.3% Fe, 25.1% O, and 1.6% S, corresponding to a formula of $\text{Fe}_3\text{O}_{3.6}\text{S}_{0.1}$, which is consistent with magnetite. The smaller grain has a composition of 76.6% Fe, and 23.1% O, corresponding to a formula of $\text{FeO}_{1.05}$, which is a ferrous oxide. Both grains appear to be secondary or partially oxidized on the outer edges.

Another example of a ferrous iron oxide is shown in Photomicrograph 21.



The grain has the composition 75.3% Fe and 23.7% O, corresponding to a formula of $\text{FeO}_{1.10}$. A small fraction of cobalt (0.9%) was also present in the phase. The morphology and composition is consistent with a sliver of partially “rusted” iron.

Barite (BaSO_4) was also identified in the sample, this combined with the absence of iron sulfides, is an indication that the redox conditions are not sulfate-reducing.

A summary of the reduced iron species identified in the samples is provided in Table 7.

Table 7 - Summary of Reduced Iron Phases in the Seneca AFB Samples Analyzed by Electron Microprobe (EMP)

Sample ID	Phases and Associations
SA1-9-11	Titanium-bearing ferrous oxide.
SA1-6-8	Magnetite and/or ferrous oxide.
SB1-7-9	Magnetite, ilmenite, and ferrous iron oxide.
SB1-7.5-9.5	Magnetite, iron metal (1 grain), and possible titanium-bearing ferrous hydroxide (1 grain).

Attachment 1 - Summary of EMP Grain Analyses

ID	Raw					Normalized to 100%					Interpreted Phase
	%Fe	%O	%Ti	%S	Total	%Fe-N	%O-N	%Ti-N	%S-N	Total-N	
C1-A_1	46.51	0.7941	NA	44.96	92.26	50.41	0.8607	NA	48.73	100	7 µm Framboidal Pyrite (FeS ₂)
C3-A_2	45.99	1.0842	NA	47.9	94.97	48.42	1.1416	NA	50.43	100	1 µm Granular Pyrite (FeS ₂)
C4-A_2	48.1	0.6757	NA	46.07	94.85	50.72	0.7124	NA	48.57	100	25 µm Framboidal Pyrite (FeS ₂)
C6-A_6	30.23	4.65	NA	38.2	73.09	41.37	6.37	NA	52.27	100	1 µm Patially Ox.? Pyrite (FeS ₂)
C6-A_7	44.33	2.0009	NA	40.5	86.84	51.05	2.3041	NA	46.64	100	17 µm Framboidal Pyrite (FeS ₂)
C6-A_7a	291.77	24.34	NA	333.58	649.69	44.91	3.75	NA	51.34	100	Rejected- Low Cup Current
C6-A_7b	42.73	2.6991	NA	44.54	89.96	47.49	3	NA	49.51	100	17 µm Framboidal Pyrite (FeS ₂)
C7-A_1	44.67	1.55	NA	46.15	92.37	48.36	1.678	NA	49.96	100	2 µm Granular Pyrite (FeS ₂)
C7-A_3	66.55	27.42	NA	0	93.97	70.82	29.18	NA	0	100	3x10 µm Ti-Magnetite (Fe ₃ O ₄)
C11-A_3	72.4	24.47	NA	0	96.87	74.74	25.26	NA	0	100	35 µm Crystalline Magnetite (Fe ₃ O ₄)
C11-A_4	71.87	22.08	NA	0.0084	93.96	76.49	23.5	NA	0.0089	100	40 µm Crystalline Magnetite (Fe ₃ O ₄)
C11-A_5	4.08	0.4502	NA	0.9438	5.48	74.55	8.22	NA	17.23	100	50x150 µm Mineralized Organic C
C13-A_1	70.9	22.61	NA	0.0074	93.52	75.82	24.18	NA	0.0079	100	8 µm Crystalline Magnetite (Fe ₃ O ₄)
C13-A_2	67.43	26.9	NA	0.0031	94.33	71.48	28.51	NA	0.0033	100	2 µm Crystalline Magnetite (Fe ₃ O ₄)
C13-A_4	52.13	19.43	NA	0.116	71.67	72.73	27.11	NA	0.1619	100	1 µm Crystalline Magnetite (Fe ₃ O ₄)
C13-A_6	72.49	24.74	NA	0.005	97.24	74.55	25.44	NA	0.0052	100	5 µm Crystalline Magnetite (Fe ₃ O ₄)
C13-A_7	71.38	24.49	NA	0	95.87	74.45	25.55	NA	0	100	5 µm Crystalline Magnetite (Fe ₃ O ₄)
C13-A_8	71.99	25.69	NA	0	97.68	73.7	26.3	NA	0	100	20 µm Crystalline Magnetite (Fe ₃ O ₄)
C15-A_1	69.67	24.91	NA	0.0123	94.59	73.65	26.33	NA	0.013	100	Crystalline Magnetite (Fe ₃ O ₄)
C15-A_2	65.4	25.07	NA	0.063	90.53	72.24	27.69	NA	0.0696	100	6 µm Magnetite (Fe ₃ O ₄)
C15-A_3	53.93	20.23	NA	0.6689	74.83	72.07	27.03	NA	0.8939	100	Crystalline Magnetite (Fe ₃ O ₄)
C15-A_3b	99.5	0.4693	NA	0.0172	99.99	99.51	0.4693	NA	0.0172	100	4x12 µm Iron Metal (Fe)
C15-A_3c	71.47	25.67	NA	0.0261	97.16	73.55	26.42	NA	0.0268	100	5 µm Spherical Magnetite (Fe ₃ O ₄)
C15-A_4a	59.98	23.37	NA	0.1607	83.51	71.83	27.98	NA	0.1925	100	1 µm Magnetite (Fe ₃ O ₄)
C15-A_5a	69.95	25.8	NA	0.0042	95.75	73.06	26.94	NA	0.0044	100	12 µm Magnetite (Fe ₃ O ₄)
B3_1-1_1a	44.88	2.4117	NA	48.25	95.54	46.97	2.5244	NA	50.5	100	7 µm Framboidal Pyrite (FeS ₂)
B3_1-1_3a	72.23	21.76	NA	0.008	94	76.84	23.15	NA	0.0085	100	200 µm Crystalline Magnetite (Fe ₃ O ₄) coated with iron disulfide.
B3_1-1_4a	47.11	13.36	NA	22.9	83.37	56.51	16.03	NA	27.47	100	110 µm Oxidized Pyrite or GR?
B3_3-1_1	72.12	26.89	NA	0	99.01	72.84	27.16	NA	0	100	250 µm Crystalline Magnetite (Fe ₃ O ₄)
B3_3-1_2	49.1	1.2552	NA	46.83	97.18	50.52	1.2916	NA	48.19	100	1 µm Granular Pyrite (FeS ₂) in 60 µm cluster
B3_3-1_3	56.79	23.31	NA	5.88	85.98	66.04	27.11	NA	6.84	100	Green Rust? 1-6 µm rind
B3_3-1_3b	55.34	17.65	NA	9.22	82.21	67.32	21.47	NA	11.21	100	Green Rust? 1-7 µm rind
B3_3-1_3c	5.04	4.53	NA	2.1507	11.72	43.02	38.63	NA	18.35	100	Mineralized Organic C
B3_3-1_4	53.3	15.6	NA	10.5	79.4	67.13	19.64	NA	13.23	100	Green Rust?
B3_3-1_4b	71.18	26.5	NA	0.0069	97.69	72.87	27.12	NA	0.0071	100	Crystalline Magnetite (Fe ₃ O ₄)
B3_3-1_4c	44.96	2.9714	NA	41.71	89.64	50.16	3.31	NA	46.53	100	1 µm Granular Pyrite (FeS ₂)
B3_3-1_6a	14.73	11.15	NA	9.28	35.16	41.89	31.71	NA	26.4	100	Mineralized Organic C >100 µm x 20 µm

ID	%Fe	%O	%Ti	%S	Total	%Fe-N	%O-N	%Ti-N	%S-N	Total-N	Interpreted Phase
B3_5-1_1	41.86	2.5835	NA	39.56	84	49.83	3.08	NA	47.1	100	1 µm Granular Pyrite (FeS ₂)
B3_5-1_4	41.83	1.3097	NA	42.18	85.32	49.03	1.5349	NA	49.44	100	25 µm Framboidal Pyrite (FeS ₂)
B3_7-1_1	33.31	11.52	NA	13.77	58.6	56.85	19.65	NA	23.5	100	Green Rust? 1-10 µm rind
B3_7-1_4	69.71	26.52	NA	0	96.23	72.44	27.56	NA	0	100	>100 µm Crystalline Hematite (Fe ₂ O ₃) or Magnetite (Fe ₃ O ₄) w/iron disulfide coating
DTSB-1-10_1	41.96	4.69	0.0926	41	87.73	47.82	5.34	0.1056	46.73	100	6 µm partially oxidized pyrite or possibly pyrrhotite (FeS _{1.7} O _{0.4})
DTSB-1-10_2	17.91	17.62	0.0024	0.0471	35.58	50.35	49.52	0.0068	0.1325	100	Ca-Mg-Fe Carbonate
DTSB-1-10_3	61.63	25.49	0.3073	0.0398	87.47	70.46	29.14	0.3513	0.0456	100	Amorphous 12 µm hematite (Fe ₂ O _{2.9}) or magnetite (Fe ₃ O _{4.3})
DTSB-1-10_4a	51.88	34.2	0.0874	0.0254	86.2	60.19	39.68	0.1014	0.0295	100	Iron silicate (FeSi _{0.5} O _{2.3})
DTSB-1-10_4b	42.19	33.91	0.1311	0.02	76.25	55.33	44.48	0.1719	0.0262	100	Reanalysis - Iron silicate (FeSi _{1.1} O _{2.8})
DTSB-1-10_5	52.54	33.22	0.0737	0.0223	85.86	61.19	38.7	0.0858	0.0259	100	10 µm x 20 µm hydrous ferrous hydroxide (Fe(OH) ₂ ·0.2H ₂ O)
DTSB-1-10_6	41.28	4.48	0.0545	41.35	87.16	47.36	5.13	0.0625	47.44	100	5 µm partially oxidized pyrite (FeS _{1.7} O _{0.4})
DTSB-1-10_7	0.0008	0.001	0	0.0003	0	39.83	47.75	0	12.42	100	Rejected-Vacuum leak
DTSB-1-10_7	24.29	32.85	0.0492	0.0208	57.2	42.46	57.42	0.0859	0.0363	100	Reanalysis, hydrous ferric hydroxide (Fe(OH) ₃ ·1.7H ₂ O) or hydrous ferrous hydroxide (Fe(OH) ₂ ·2.7H ₂ O)
DTSB-1-17_1	53.67	20.26	0.0546	14.98	88.96	60.33	22.77	0.0614	16.84	100	Partially oxidized iron monosulfide (FeS _{0.5} O _{1.3})
DTSB-1-17_2	64.55	30.94	0.9041	0.0089	96.41	66.96	32.09	0.9378	0.0092	100	Ferrous oxide (FeO _{1.2})
DTSB-1-17_3	33.7	34.75	29.96	0	98.41	34.24	35.32	30.44	0	100	Very porous hydrated ilmenite (FeTiO ₃ ·0.6H ₂ O)
DTSB-1-17_4	45.99	1.917	0.0517	43.23	91.19	50.44	2.1023	0.0567	47.4	100	5 µm partially oxidized pseudoframboidal pyrite (FeS _{1.6} O _{0.1})
DTSB-1-17_6	58.05	31.98	0.0555	0.105	90.19	64.37	35.46	0.0615	0.1164	100	Ferrous hydroxide (Fe(OH) _{1.9})
DTSB-1-17_7	46.73	2.6315	0.0698	44.36	93.79	49.83	2.8057	0.0744	47.29	100	Partially oxidized pyrite (FeS _{1.7} O _{0.2})
DTSB-1-17_8	63.56	34.1	0.1989	0.6168	98.47	64.54	34.63	0.202	0.6264	100	Ferrous hydroxide (Fe(OH) _{1.9})
DTSB-17_1	41.97	3.44	0	37.89	83.3	50.38	4.13	0	45.49	100	10 µm partially oxidized pyrite (FeS _{1.6} O _{0.3})
DTSB-17_2	41.96	4.71	0	38.05	84.71	49.53	5.56	0	44.91	100	12 µm partially oxidized pyrite (FeS _{1.6} O _{0.4})
DTSB-17_3a	39.21	14.13	0	0	53.34	73.51	26.49	0	0	100	Gray part of 180 µm grain - iron-titanium oxide (FeTi _{1.5} O _{1.3})
DTSB-17_3b	60.82	28.6	9.12	0	98.54	61.72	29.02	9.26	0	100	White part of 180 µm grain - titanomagnetite (Fe ₂ Ti _{0.3} O _{3.3})
DTSB-17_3c	39.12	29.7	27.26	0	96.09	40.71	30.91	28.37	0	100	Reanalysis of gray part of 180 µm grain - ilmenite (FeTi _{0.8} O _{2.7})
DTSB-17_4a	42.45	9.44	0.0177	18.46	70.38	60.33	13.41	0.0251	26.24	100	2 µm partially oxidized iron monosulfide (FeS _{0.8} O _{0.8})
DTSB-17_4b	46.52	9.52	0.0425	19.82	75.9	61.28	12.54	0.056	26.12	100	Reanalysis of 2 µm partially oxidized iron monosulfide (FeS _{0.7} O _{0.7})

ID	%Fe	%O	%Ti	%S	Total	%Fe-N	%O-N	%Ti-N	%S-N	Total-N	Interpreted Phase
DTSB-17_5	33.06	8.42	0.0412	29.45	70.97	46.58	11.86	0.058	41.5	100	Partially oxidized pyrite or possibly pyrrhotite (FeS _{1.6} O _{0.9})
DTSB-17_6	31.38	7.62	0.0411	27.85	66.89	46.92	11.39	0.0615	41.63	100	2-3 µm partially oxidized pyrite or possibly pyrrhotite (FeS _{1.6} O _{0.9})
DTSB-17_7	45.83	9.58	0.0455	19.87	75.32	60.84	12.71	0.0605	26.39	100	8 µm partially oxidized iron monosulfide (FeS _{0.8} O _{0.7})
DTSB-17_8	46.57	9.51	0.0643	20.49	76.63	60.76	12.41	0.0839	26.74	100	16 x 10 µm partially oxidized iron monosulfide (FeS _{0.8} O _{0.7})
DTSB-17_9	40.43	3.8	0.0584	34.85	79.14	51.09	4.8	0.0738	44.04	100	Partially oxidized pyrite or possibly pyrrhotite (FeS _{1.5} O _{0.3})
DTSB-3-10_1	0.1307	35.43	55.75	0	91.31	0.1432	38.8	61.06	0	100	20 µm rutile (TiO _{1.9})
DTSB-3-10_2	25.31	28.97	22.27	0	76.55	33.06	37.85	29.09	0	100	Iron-titanium-aluminum silicate (FeTiSi _{1.8} O ₄). Si determined by difference as Al and Si were not part of analysis
DTSB-3-10_4	45.57	31.76	14.95	0	92.28	49.38	34.42	16.2	0	100	15 µm secondary titano-ferrous iron oxyhydroxide (FeTi _{0.4} O _{1.1} (OH) _{1.3})
DTSB-3-10_5	38.58	28.95	28.81	0	96.34	40.05	30.05	29.91	0	100	Primary 170 µm ilmenite (FeTi _{0.9} O _{2.6})
DTSB-3-10_6	69.09	25.59	0.1325	0.0013	94.82	72.87	26.99	0.1398	0.0014	100	Primary 100 µm iron oxide, possible hematite (Fe ₂ O _{2.6})
DTSB-3-10_7	34.29	29.65	26.62	0	90.55	37.87	32.74	29.39	0	100	Primary 170 µm ilmenite (FeTi _{0.9} O _{3.0})
DTSB-3-10_9a	48.18	8.74	0.0823	22.08	79.09	60.92	11.05	0.1041	27.92	100	Partially oxidized iron 40 µm monosulfide (FeS _{0.8} O _{0.6})
DTSB-3-10_9b	42.13	27.73	0.0716	0.0458	69.97	60.2	39.63	0.1023	0.0655	100	Iron silicate coating quartz (FeSi _{1.4} O _{2.3}). Si by difference.
DTSB-3-16_1	20.17	17.82	0.0234	9.85	47.86	42.14	37.23	0.0489	20.58	100	5 µm FeSiSO
DTSB-3-16_10	43.15	5.09	0.0673	41.55	89.87	48.02	5.67	0.0748	46.24	100	10 µm x 30 µm partially oxidized pyrite (FeS _{1.7} O _{0.4})
DTSB-3-16_2	32.07	30.32	0.0205	0.0724	62.48	51.32	48.53	0.0328	0.1159	100	13 µm FePO
DTSB-3-16_4	29.87	24.4	3.32	0	57.58	51.87	42.37	5.76	0	100	Hydrous titano-ferrous oxyhydroxide (FeTi _{0.1} (OH) _{1.2} O _{0.7} -H ₂ O) or titano-ferric oxyhydroxide (FeTi _{0.1} (OH) _{2.2} O _{0.7})
DTSB-3-16_5	15.4	14.51	0.0302	11.53	41.47	37.13	34.99	0.0729	27.8	100	25 µm FeSiSO(Al)
DTSB-3-16_6a	15.03	27.1	9.92	0	52.06	28.88	52.06	19.06	0	100	Rejected-Out of focus
DTSB-3-16_6b	18.17	27.03	11.28	0	56.48	32.17	47.86	19.97	0	100	Reanalysis, hydrated ilmenite? (FeTi _{0.7} O _{2.4} ·2.8H ₂ O) or partially oxidized ilmenite
DTSB-3-16_8	30.16	28.11	0.0265	0.194	58.5	51.56	48.06	0.0452	0.3316	100	Ferric hydroxide (Fe(OH) _{3.3}) or hydrous ferrous hydroxide (Fe(OH) ₂ ·1.3H ₂ O)
DTSB-3-16_9	34.6	30.72	27.63	0	92.95	37.23	33.04	29.73	0	100	Ilmenite (FeTi _{0.9} O _{3.1})
DTSB-6-10_1	48.81	20.98	0.0433	4.5	74.33	65.67	28.22	0.0583	6.05	100	10 x 30 µm grain - ferrous oxysulfate? (Fe(SO ₄) _{0.16} O _{0.85})
DTSB-6-10_2	42.4	10.17	0.0837	18.08	70.74	59.94	14.38	0.1183	25.56	100	8 µm partially oxidized iron monosulfide (FeS _{0.8} O _{0.8})

ID	%Fe	%O	%Ti	%S	Total	%Fe-N	%O-N	%Ti-N	%S-N	Total-N	Interpreted Phase
DTSB-6-10_3	49.25	8.47	0.0203	24.83	82.57	59.65	10.26	0.0245	30.07	100	5 x 10 µm partially oxidized iron monosulfide (FeS _{0.9} O _{0.6})
DTSB-6-10_5	45.26	16.5	0.0615	22.46	84.29	53.7	19.58	0.073	26.64	100	90 µm partially oxidized iron monosulfide (FeS _{0.9} O _{1.3})
DTSB-8-10_1	44.33	9.25	0.0549	20.77	74.4	59.58	12.43	0.0738	27.91	100	8 µm partially oxidized iron monosulfide (FeS _{0.8} O _{0.7})
DTSB-8-10_2	36.59	6.79	0.0751	34.47	77.93	46.96	8.71	0.0963	44.23	100	Partially oxidized pyrite or possibly pyrrhotite (FeS _{1.6} O _{0.7})
DTSB-8-10_3	37.55	4.13	0.0652	35.4	77.15	48.68	5.36	0.0845	45.88	100	Partially oxidized pyrite or possibly pyrrhotite (FeS _{1.7} O _{0.4})
DTSB-8-10_4	42.46	3.86	0.0586	37.98	84.36	50.33	4.58	0.0694	45.02	100	7 µm partially oxidized pyrite or possibly pyrrhotite (FeS _{1.6} O _{0.3})
DTSB-8-10_5	44.94	5	0.0532	36.43	86.43	52	5.78	0.0616	42.15	100	Partially oxidized pyrite or possibly pyrrhotite (FeS _{1.4} O _{0.4})
DTSB-8-10_6	45.58	4.63	0.0842	39.57	89.86	50.72	5.15	0.0937	44.04	100	Partially oxidized pyrite or possibly pyrrhotite (FeS _{1.5} O _{0.4})
DTSB-8-17_1	56.5	4.93	0.0521	29.33	90.82	62.22	5.43	0.0573	32.29	100	20 µm partially oxidized iron monosulfide (FeS _{0.8} O _{1.3})
DTSB-8-17_2	40.05	15.39	0.0593	19.35	74.85	53.51	20.56	0.0792	25.85	100	12 µm partially oxidized iron monosulfide (FeS _{0.8} O _{1.3})
DTSB-8-17_3a	52.73	7.81	0.0322	24.44	85.01	62.02	9.19	0.0379	28.75	100	18 µm partially oxidized iron monosulfide (FeS _{0.8} O _{0.5})
DTSB-8-17_3b	47.33	7.87	0.0339	22.08	77.31	61.22	10.17	0.0439	28.56	100	Partially oxidized iron monosulfide (FeS _{0.8} O _{0.6}). Same grain as above, different spot
DTSB-8-17_4	38.4	43.07	0.9232	0.4813	82.87	46.33	51.97	1.114	0.5808	100	Hydrous ferric hydroxide (Fe(OH) ₃ ·0.9H ₂ O), hydrous ferrous hydroxide (Fe(OH) ₂ ·1.9H ₂ O), or hydroxy green rust ([Fe ^{II} _(1-x) Fe ^{III} _x (OH) ₂] ^{x+} ·[xOH ⁻ ·mH ₂ O] ^{x-}). In a mass associated with iron silicate and organic C.
DTSB-8-17_5	45.19	8.86	0.0597	20.17	74.27	60.84	11.93	0.0804	27.15	100	3 µm partially oxidized iron monosulfide (FeS _{0.8} O _{0.6})
DTSB-8-17_6	38.4	11.12	0.0669	18.28	67.87	56.58	16.38	0.0986	26.94	100	10 x 40 µm partially oxidized iron monosulfide (FeS _{0.8} O _{1.0})
UTSB-16-10_2	17.09	26.89	10.17	0	54.16	31.56	49.66	18.78	0	100	35 µm x 50 µm Hydrous ilmenite? (FeTi _{0.7} O _{2.4} ·3.1H ₂ O) or partially oxidized ilmenite or both
UTSB-16-10_4a	14.6	9.77	0.0346	25.34	49.75	29.35	19.64	0.0696	50.94	100	11 µm partially oxidized pyrite? (FeS _{3.1} O _{2.4})
UTSB-16-10_4b	14.23	9.51	0.0347	25.89	49.67	28.66	19.14	0.0699	52.13	100	Reanalysis of 11 µm partially oxidized pyrite? (FeS _{2.3} O _{3.2})
UTSB-16-10_5	11.35	7.5	0.0513	39.79	58.69	19.34	12.77	0.0874	67.8	100	3 µm partially oxidized iron sulfide? (FeS _{6.1} O _{2.3})

ID	%Fe	%O	%Ti	%S	Total	%Fe-N	%O-N	%Ti-N	%S-N	Total-N	Interpreted Phase
UTSB-16-10_6	15.06	15.53	0.0173	18.27	48.89	30.81	31.78	0.0355	37.38	100	7 µm partially oxidized pyrite? (FeS _{2.1} O _{3.6})
97FD-0090_2	66.29	29.83	2.9691	0	99.09	66.9	30.1	2.9964	0	100	Titanium-bearing hematite (Fe ₂ Ti _{0.1} O _{3.1})
97FD-0090_3	67.82	29.01	1.8339	0	98.67	68.74	29.4	1.8587	0	100	Titanium-bearing hematite (Fe ₂ Ti _{0.06} O _{3.0}), with euhedral inclusions. Appears to be a weathering product.
97FD-0090_4	59.61	34.26	8.06	0	101.93	58.48	33.62	7.91	0	100	Titaniferrous hydroxide (FeTi _{0.2} (OH) _{2.0}). Secondary morphology.
97FD-0090_5	0.4288	5.16	0.1958	11.04	16.83	2.5479	30.67	1.1631	65.62	100	Partially oxidized lead sulfide (PbS _{0.9} O _{0.8})
97FD-0090_6	60.09	30.42	5.67	0	96.18	62.48	31.62	5.9	0	100	Titanium-bearing hematite (Fe ₂ Ti _{0.2} O _{3.5}) or titaniferrous hydroxide (FeTi _{0.1} (OH) _{1.77})
97FD-0090_7	57.28	31.94	7.75	0	96.97	59.07	32.94	7.99	0	100	Titaniferrous hydroxide (FeTi _{0.2} (OH) _{2.0})
97FD-0090_8	65.47	31.44	3.15	0	100.06	65.43	31.42	3.15	0	100	Titanium-bearing hematite (Fe ₂ Ti _{0.1} O _{3.4}) or titaniferrous hydroxide (FeTi _{0.06} (OH) _{1.7})
97FD-0090_9	69.75	30.65	1.0478	0	101.44	68.76	30.21	1.0329	0	100	Titanium-bearing hematite (Fe ₂ Ti _{0.04} O _{3.1})
97S-0086_1	0.403	17.43	0.0701	21.02	38.93	1.0352	44.78	0.1801	54	100	Partially oxidized zinc sulfide (ZnS _{0.7} O _{1.2})
97S-0086_3	53.33	32.25	6.03	0	91.61	58.21	35.2	6.58	0	100	Titaniferrous hydroxide (FeTi _{0.1} (OH) _{2.1})
97S-0086_4a	59.5	29.06	6.67	0	95.23	62.48	30.52	7	0	100	Titanium-bearing hematite (Fe ₂ Ti _{0.3} O _{3.4}) or titaniferrous hydroxide (FeTi _{0.1} (OH) _{1.7})
97S-0086_4b	59.9	29.07	6.65	0	95.62	62.65	30.4	6.96	0	100	Titanium-bearing hematite (Fe ₂ Ti _{0.3} O _{3.4}) or titaniferrous hydroxide (FeTi _{0.1} (OH) _{1.7})
97S-0086_5	65.69	29.58	4.75	0	100.02	65.68	29.57	4.75	0	100	Titanium-bearing hematite (Fe ₂ Ti _{0.2} O _{3.1})
97S-0087_2	42.35	34.98	3.76	0	81.09	52.22	43.14	4.64	0	100	Titaniferrous hydroxide? (FeTi _{0.1} (OH) _{2.9}) or hydrated titaniferrous hydroxide? (FeTi _{0.1} (OH) _{2.3} ·0.6 H ₂ O)
97S-0087_3	43.05	29.84	1.6232	0	74.51	57.78	40.04	2.1787	0	100	Hydrated titaniferrous hydroxide (FeTi _{0.04} (OH) _{2.2} ·0.2 H ₂ O)
97S-0087_4	38.5	29.96	3.58	0	72.05	53.44	41.59	4.97	0	100	Hydrated titaniferrous hydroxide (FeTi _{0.1} (OH) _{2.4} ·0.3 H ₂ O)
97S-0087_5	41.03	29.63	0.4281	0.0044	71.09	57.71	41.68	0.6022	0.0062	100	Ferrous-ferric hydroxide mix (Fe(OH) _{2.5}). Hydroxy green rust?
97S-0087_6	32.62	28.91	0.4138	0	61.94	52.67	46.66	0.668	0	100	Ferric hydroxide (Fe(OH) _{3.1}). Hydroxy green rust?
97S-0088_1	67.33	30.07	2.4913	0	99.89	67.4	30.1	2.4939	0	100	Hematite? (Fe ₂ Ti _{0.1} O _{3.1})
97S-0088_10	60.21	30.47	8.06	0	98.73	60.98	30.86	8.16	0	100	Titanium-bearing ferric oxide (FeTi _{0.2} O _{1.8})
97S-0088_3	56.54	24.25	0.084	0.171	81.05	69.76	29.93	0.1037	0.211	100	2 µm hematite (Fe _{2.0} O _{3.0})
97S-0088_4	62.57	31.72	3.13	0	97.42	64.23	32.56	3.21	0	100	Titanium-bearing hematite (Fe ₂ Ti _{0.1} O _{3.5}) or titaniferrous hydroxide (FeTi _{0.1} (OH) _{1.77})
97S-0088_7	62.13	34.76	4.55	0	101.44	61.25	34.27	4.49	0	100	Titaniferrous hydroxide (FeTi _{0.1} (OH) _{2.0})
97S-0088_8	64.03	31.35	2.4198	0.0119	97.82	65.46	32.05	2.4738	0.0122	100	Titanium-bearing hematite (Fe ₂ Ti _{0.1} O _{3.4}) or titaniferrous hydroxide (FeTi _{0.04} (OH) _{1.7})

ID	%Fe	%O	%Ti	%S	Total	%Fe-N	%O-N	%Ti-N	%S-N	Total-N	Interpreted Phase
97S-0089_1a	56.43	31.19	2.9077	0	90.53	62.33	34.45	3.21	0	100	Titaniferrous hydroxide ($\text{FeTi}_{0.1}(\text{OH})_{1.9}$)
97S-0089_1b	36.69	34.1	18.44	0	89.23	41.11	38.22	20.67	0	100	Darker part of grain above, partially oxidized ilmenite? ($\text{FeTi}_{0.6}\text{O}_{3.2}$)
97S-0089_2	56.62	28.37	5.72	0	90.71	62.42	31.28	6.3	0	100	Titaniferrous hydroxide ($\text{FeTi}_{0.1}(\text{OH})_{1.8}$)
97S-0089_4	37.61	31.4	5.67	0	74.68	50.36	42.04	7.6	0	100	Titaniferrous hydroxide? ($\text{FeTi}_{0.2}(\text{OH})_{2.9}$) or hydrated titaniferrous hydroxide? ($\text{FeTi}_{0.2}(\text{OH})_{2.7} \cdot 0.2 \text{H}_2\text{O}$)
97S-0089_5	53.43	31.75	2.4463	0	87.62	60.98	36.23	2.792	0	100	Titaniferrous hydroxide ($\text{FeTi}_{0.05}(\text{OH})_{2.1}$)
97S-0089_6	42.54	41.2	8.12	0	91.85	46.31	44.85	8.84	0	100	Titaniferrous hydroxide? ($\text{FeTi}_{0.2}(\text{OH})_{3.4}$) or hydrated titaniferrous hydroxide? ($\text{FeTi}_{0.2}(\text{OH})_{2.7} \cdot 0.7 \text{H}_2\text{O}$)
97S-0089_7a	57.6	32.83	1.7842	0	92.21	62.46	35.6	1.935	0	100	Titaniferrous hydroxide ($\text{FeTi}_{0.04}(\text{OH})_{2.0}$)
97S-0089_7b	25.59	38.31	31.28	0	95.18	26.89	40.25	32.86	0	100	Different phase in same grain as above, hydrated ferrous iron-titanium oxide ($\text{FeTi}_{1.4}\text{O}_{3.8} \cdot 1.4 \text{H}_2\text{O}$) or hydrated ferric iron-titanium oxide ($\text{FeTi}_{1.4}\text{O}_{4.3} \cdot 0.9 \text{H}_2\text{O}$)
97S-0090_2	57.09	32.03	4.89	0	94.01	60.73	34.07	5.2	0	100	Titaniferrous hydroxide ($\text{FeTi}_{0.1}(\text{OH})_{2.0}$)
97S-0090_3a	40.22	34.06	20.16	0	94.44	42.59	36.06	21.35	0	100	Ilmenite? ($\text{FeTi}_{0.6}\text{O}_{3.0}$)
97S-0090_3b	64.93	32.76	1.9077	0	99.59	65.19	32.89	1.9155	0	100	Titanium-bearing hematite ($\text{Fe}_2\text{Ti}_{0.06}\text{O}_{3.5}$) or titaniferrous hydroxide ($\text{FeTi}_{0.03}(\text{OH})_{1.76}$)
97S-0090_4	54.68	29.34	4.7	0	88.71	61.63	33.07	5.29	0	100	Titanium-bearing hematite ($\text{Fe}_2\text{Ti}_{0.2}\text{O}_{3.1}$)
97S-0090_5a	56.99	29.52	7.68	0	94.19	60.51	31.34	8.15	0	100	Titaniferrous hydroxide ($\text{FeTi}_{0.2}(\text{OH})_{1.8}$)
97S-0090_5b	56.18	33.35	6.31	0	95.85	58.61	34.8	6.59	0	100	Titaniferrous hydroxide ($\text{FeTi}_{0.1}(\text{OH})_{2.1}$)
97S-0090_6	54.08	27.7	0.3052	6.94	89.03	60.75	31.11	0.3429	7.8	100	Ferrous, lead-bearing oxyhydroxysulfate ($\text{FePb}_{0.05}(\text{SO}_4)_{0.2}\text{O}_{0.7}(\text{OH})_{0.3}$)
97S-0090_7	58.45	29.79	3.59	0	91.83	63.66	32.44	3.91	0	100	Titaniferrous hydroxide ($\text{FeTi}_{0.07}(\text{OH})_{1.8}$)
97S-0091_1	68.08	30.85	1.6033	0	100.53	67.72	30.68	1.5949	0	100	Titanium-bearing hematite ($\text{Fe}_2\text{Ti}_{0.06}\text{O}_{3.2}$) or titaniferrous hydroxide ($\text{FeTi}_{0.03}(\text{OH})_{1.6}$)
97S-0091_2	61.1	30.11	6.76	0	97.96	62.36	30.73	6.9	0	100	Titanium-bearing hematite ($\text{Fe}_2\text{Ti}_{0.2}\text{O}_{3.4}$) or titaniferrous hydroxide ($\text{FeTi}_{0.1}(\text{OH})_{1.7}$)
97S-0091_3	61.81	28.97	5.9	0	96.68	63.93	29.97	6.1	0	100	Titanium-bearing hematite ($\text{Fe}_2\text{Ti}_{0.2}\text{O}_{3.3}$) or titaniferrous hydroxide ($\text{FeTi}_{0.1}(\text{OH})_{1.6}$)
97S-0091_4	64.99	28.66	1.907	0	95.56	68.01	29.99	1.9957	0	100	Titanium-bearing hematite ($\text{Fe}_2\text{Ti}_{0.06}\text{O}_{3.1}$) with hematite parting.
97S-0091_5	61.84	29.89	5.22	0	96.95	63.78	30.83	5.38	0	100	Titanium-bearing hematite ($\text{Fe}_2\text{Ti}_{0.2}\text{O}_{3.4}$) or titaniferrous hydroxide ($\text{FeTi}_{0.1}(\text{OH})_{1.7}$)
97S-0091_6	70.9	27.84	0.6081	0	99.35	71.37	28.02	0.6121	0	100	Magnetite ($\text{Fe}_3\text{O}_{4.1}$)
SA1-6-8_1a	66.85	22.89	0.0612	1.4461	91.25	73.26	25.09	0.0671	1.5848	100	Magnetite? ($\text{Fe}_3\text{O}_{3.6}\text{S}_{0.1}$)
SA1-6-8_1b	67.51	20.32	0.0461	0.1066	87.99	76.73	23.1	0.0524	0.1212	100	Reanalysis of above, ferrous oxide ($\text{FeO}_{1.0}$)
SA1-6-8_3	62.37	27.89	3.97	0	94.24	66.18	29.6	4.22	0	100	Titanium-bearing hematite ($\text{Fe}_2\text{Ti}_{0.2}\text{O}_{3.1}$)

ID	%Fe	%O	%Ti	%S	Total	%Fe-N	%O-N	%Ti-N	%S-N	Total-N	Interpreted Phase
SA1-6-8_5	59.84	24.08	0.288	0.0899	84.29	70.99	28.56	0.3417	0.1067	100	Magnetite (Fe ₃ O _{4.2})
SA1-911_4a	66.03	24.52	0.025	0	90.58	72.9	27.08	0.0276	0	100	Iron-titanium oxide (FeTi _{0.2} O _{1.3})
SA1-911_4b	69.8	23.61	0.0055	0	93.42	74.72	25.28	0.0059	0	100	Iron-titanium oxide (FeTi _{0.1} O _{1.2})
SA1-911_4c	68.85	24.24	0	0	93.09	73.96	26.04	0	0	100	Iron-titanium oxide (FeTi _{0.1} O _{1.2})
SA1-911_5	53.6	30.19	0.0333	0.0241	83.85	63.93	36.01	0.0397	0.0288	100	Iron-aluminum silicate (FeSi _{0.6} O ₂). Note: Al not analyzed. Si determined by difference
SA1-911_6	41.38	12.3	0	0	53.68	77.09	22.91	0	0	100	Iron-titanium oxide (FeTi _{1.3} O _{1.0}). Note Ti determined by difference.
SA1-911_7	0.083	38.29	0	6.55	44.93	0.1847	85.23	0	14.59	100	Barite
SB1-7.5-9.5_1a	34.74	1.0405	0.0293	0.0137	35.83	96.98	2.9043	0.0818	0.0381	100	Iron metal with minor oxidation (FeO _{0.10}) - Grain off-center.
SB1-7.5-9.5_1b	64.3	0.9906	0.0454	0.0178	65.35	98.39	1.5158	0.0695	0.0272	100	Reanalysis of above, Iron metal with minor oxidation (FeO _{0.05})
SB1-7.5-9.5_2	57.5	29.09	8.01	0	94.61	60.78	30.75	8.47	0	100	Titanium-bearing hematite (Fe ₂ Ti _{0.2} O _{3.5}) or titaniferrous hydroxide (FeTi _{0.2} (OH) _{1.8})
SB1-7.5-9.5_3	71.63	25.28	0.1913	0.0015	97.1	73.77	26.04	0.197	0.0016	100	Magnetite (Fe ₃ O _{3.7})
SB1-7.5-9.5_5	67.55	27.4	0.1825	0.0096	95.14	71	28.8	0.1918	0.0101	100	Magnetite (Fe ₃ O _{4.3})
SB1-7-9_1	72.83	24.95	0.0967	0.0015	97.88	74.41	25.49	0.0988	0.0016	100	Magnetite (Fe ₃ O _{3.6})
SB1-7-9_2	73.27	24.59	0.0824	0.0049	97.94	74.81	25.1	0.0841	0.005	100	Magnetite (Fe ₃ O _{3.5})
SB1-7-9_3	75.29	23.72	0.0736	0.0057	99.09	75.98	23.94	0.0743	0.0057	100	Porous 450 µm x 120 µm ferrous iron oxide (FeO _{1.1})
SB1-7-9_4	36.4	30.65	28.92	0	95.97	37.93	31.93	30.14	0	100	Ilmenite (FeTi _{0.9} O _{2.9})
SB1-7-9_5	39.01	29.71	26.15	0	94.87	41.12	31.31	27.57	0	100	Ilmenite (FeTi _{0.8} O _{2.7})
SB1-7-9_6	69.84	25.55	0.6651	0.001	96.05	72.71	26.6	0.6925	0.0011	100	Magnetite (Fe ₃ O _{3.8})

	Iron Monosulfide Diameter (μm)
dover	2
	2
	2.5
	3
	3
	5
	5 pseudoframboid
	6
	7 12x3
	7 5x10
	7
	7
	8
	8
	8
	10
	11
	12
	12
	13 16x10
	18
	20 10x30
	20 pseudoframboid
	25 10x40
	23
	40
	90
	u
	u
	u
	u
	u
n (with size)	
n (total)	
Min	2
Max	90
Median	8
Mean	13.9
Stdev	17.5
OU-1	
C4-A_2	25 framboid
C1-A_3	6 pseudoframboid
C6-A_7b	17 framboid
C7-A_2	10 framboid
C7-A_6	30 framboid
C7-A_6	20 framboid
C4-A_1	25 framboid

[illegible]

[illegible]

[illegible]

n (framboydal)	11
n (1 micron)	142
Min	1
Max	3
Median	1
Mean	1.1
Stdev	0.3

Appendix E

Calculation Briefs

Calculation Brief

Objective

To determine the log Ksp for troilite (FeS) based on published Gibbs Free Energy of Formation data

Methodology

The log of the solubility product constant (Log Ksp) which is required within the PHREEQC model is calculated from the Gibbs Free Energy of Formation using the following equations:

The standard Free Energy of Reaction (ΔGr°) is calculated from the standard Free Energy of Formation (ΔGf°) as follows:

$$\Delta Gr^\circ = \sum \Delta Gf^\circ * n \text{ (products)} - \sum \Delta Gf^\circ * n \text{ (reactants)}$$

Where

n = the number of atoms in the reaction (the stoichiometric coefficient)

The Ksp is related to ΔGr° by;

$$\Delta Gr^\circ = -RT \ln Keq \quad (1)$$

Where,

R = The gas constant = 1.9872 cal/deg mol

T = The temperature in degrees Kelvin = 298.15 K @ 25°C

Inserting R and T, and converting ln to log gives,

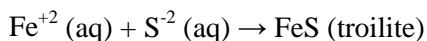
$$\Delta Gr^\circ = -1.3642 \log Ksp$$

And solving for log Ksp,

$$\log Keq = \Delta Gr^\circ / -1.3642 \quad (2)$$

Calculation

For troilite (FeS):



$$\Delta Gf^\circ (Fe^{+2}) = -18.85 \text{ kcal (Stumm and Morgan, 1981)}$$

$$\Delta Gf^\circ (S^{-2}) = 20.51 \text{ kcal (Stumm and Morgan, 1981)}$$

$$\Delta Gf^\circ \text{ (troilite)} = -24.37 \text{ kcal (Anderko and Shur, 1997)}$$

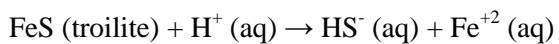
.

$$\Delta G^{\circ} = (-24.37 \times 1) - (20.51 \times 1 - 18.85 \times 1) = -26.03 \text{ kcal}$$

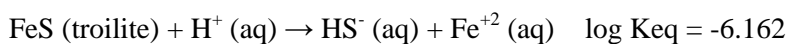
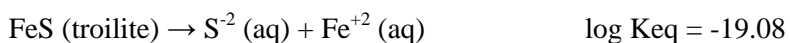
Using (2),

$$\log K_{eq} = -26.03 / -1.3642 = 19.08$$

In PHREEQC the reaction is written as;



First, the reaction is reversed, which changes the sign of Log Keq, the reaction is then added to the association reaction for bisulfide (the log K values are summed as well) to yield the equation in the proper form.



Calculation Brief

Objective

To determine the equilibrium concentration of TCE in groundwater that will result following equilibrium with biowall mulch.

Methodology

The concentration of TCE in the groundwater can not be determined directly from the K_d relationship due to the fact that adsorption of TCE onto the mulch will result in a lower TCE concentration in the groundwater once equilibrium is established. Therefore, a mass balance approach will be required. The following equations apply:

$$M_{\text{Total}} = (V_{\text{liq}} * C_{\text{liq-I}}) + (M_{\text{soil}} * C_{\text{soil-I}}) \quad (1)$$

where,

M_{Total}	=	The total mass of TCE in the system [mg]
V_{liq}	=	The volume of liquid (groundwater) in the system [L]
$C_{\text{liq-I}}$	=	The TCE concentration within the liquid (groundwater) initially [mg/L]
M_{soil}	=	The mass of mulch in the system [kg]
$C_{\text{soil-I}}$	=	The initial TCE concentration in the mulch [mg/kg] (assume 0 for the first PV)

The mass balance for the system at equilibrium (after adsorption) is given by the following;

$$M_{\text{Total}} = V_{\text{liq}} * C_{\text{liq-eq}} + M_{\text{soil}} * C_{\text{soil-eq}} \quad (2)$$

Where,

$C_{\text{liq-eq}}$	=	The TCE concentration within the liquid (groundwater) at equilibrium [mg/L]
$C_{\text{soil-eq}}$	=	The concentration of TCE in the mulch at equilibrium [mg/kg]

Because the mass of TCE in the system does not change during the adsorption, (1) and (2) can be combined to yield;

$$(V_{\text{liq}} * C_{\text{liq-I}}) + (M_{\text{soil}} * C_{\text{soil-I}}) = V_{\text{liq}} * C_{\text{liq-eq}} + M_{\text{soil}} * C_{\text{soil-eq}} \quad (3)$$

The K_d expression (which describes adsorption) is given by;

$$K_d = C_{\text{soil-eq}} / C_{\text{liq-eq}} \quad (4)$$

Solving for $C_{\text{liq-eq}}$ yields;

$$C_{\text{liq-eq}} = C_{\text{soil-eq}} / K_d \quad (5)$$

Substituting (5) into (3) yields;

$$(V_{\text{liq}} * C_{\text{liq-I}}) + (M_{\text{soil}} * C_{\text{soil-I}}) = V_{\text{liq}} * (C_{\text{soil-eq}} / K_d) + M_{\text{soil}} * C_{\text{soil-eq}} \quad (6)$$

The total soil porosity will be used to determine the soil to solution ratio (assuming complete saturation). Porosity (n) is given by;

$$n = V_{liq} / (V_{soil} + V_{liq}) \quad (7)$$

Soil volume is related to soil mass by the dry bulk density (ρ) as follows;

$$\rho = M_{soil} / (V_{soil} + V_{air}) \quad (8)$$

where,

V_{air} = The volume of air in the pore spaces of a dry soil

Because the soil is assumed to be completely saturated during the TCE adsorption,

$$V_{air} = V_{liq} \quad (9)$$

Substituting (9) into (8) and solving for ($V_{soil} + V_{liq}$) yields;

$$(V_{soil} + V_{liq}) = M_{soil} / \rho \quad (10)$$

Substituting (10) into (7) and solving for M_{soil} yields;

$$M_{soil} = (V_{liq} * \rho) / n \quad (11)$$

Substituting (11) into (6) yields;

$$(V_{liq} * C_{liq-I}) + (((V_{liq} * \rho) / n) * C_{soil-I}) = V_{liq} * (C_{soil-eq} / K_d) + ((V_{liq} * \rho) / n) * C_{soil-eq} \quad (12)$$

Distributing $C_{soil-eq}$ and dividing both sides by V_{liq} yields;

$$C_{liq-I} + (\rho / n) * C_{soil-I} = C_{soil-eq} * (1 / K_d) + (\rho / n) \quad (13)$$

Solving for $C_{soil-eq}$ yields;

$$C_{soil-eq} = (C_{liq-I} + ((\rho / n) * C_{soil-I}) / ((1 / K_d) + (\rho / n))) \quad (14)$$

As the partitioning of TCE depends on the organic carbon fraction of the soil (f_{oc}), the equilibrium constant is expressed as an organic carbon-normalized constant called K_{oc} , such that:

$$K_d = K_{oc} * f_{oc} \quad (15)$$

Substituting (15) into (14) yields:

$$C_{soil-eq} = (C_{liq-I} + ((\rho / n) * C_{soil-I}) / ((1 / (K_{oc} * f_{oc})) + (\rho / n))) \quad (16)$$

The concentration of TCE in the groundwater at equilibrium can then be determined using (5).

Calculation

An example calculation for the SS-17 site follows.

Given:

$$\begin{aligned}C_{\text{liq-I}} &= 3.930 \text{ mg/L (9/6/2007 data)} \\K_{\text{oc}} &= 21 \text{ L/kg (Shen and Wilson, 2007)} \\f_{\text{oc}} &= 0.0281 \text{ (median of analyses for C11-A, C13-A, and C15-A)} \\n &= 0.25 \\\rho &= 1.65 \text{ g/cc} = 1.65 \text{ kg/L} \\C_{\text{soil-I}} &= \text{assume 0 for first pore volume (PV)}\end{aligned}$$

Using (16) yields

$$C_{\text{soil-eq}} = (3.930 \text{ mg/L} + 0) / ((1/(21\text{L/kg} * 0.0281) + (1.65 \text{ kg/L}/0.25))) = 0.474 \text{ mg/kg}$$

The equilibrium water concentration for the first pore volume is determined using (5);

$$C_{\text{liq-eq}} = 0.474 \text{ mg/kg}/(21\text{L/kg} * 0.0281) = 0.800 \text{ mg/L} = \underline{\underline{800 \mu\text{g/L}}}$$

For the second PV

$$C_{\text{soil-I}} = 0.474 \text{ mg/kg}$$

$$C_{\text{soil-eq}} = (3.930 \text{ mg/L} + (0.474 \text{ mg/kg} * (1.65 \text{ kg/L}/0.25))) / ((1/(21\text{L/kg} * 0.0281) + (1.65 \text{ kg/L}/0.25))) = 0.851 \text{ mg/kg}$$

$$C_{\text{liq-eq}} = 0.851 \text{ mg/kg}/(21\text{L/kg} * 0.0281) = 1.440 \text{ mg/L} = \underline{\underline{1,440 \mu\text{g/L}}}$$

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Calculation Brief

Objective

To determine the contribution of dissolved sulfide to the AVS analysis. As AVS is typically performed on wet samples to avoid oxidation during drying, aqueous sulfide is included in the AVS analysis.

Methodology

$$M_{S-2-soln} = C_{S-2} * V_{soln} \quad (1)$$

Where,

$M_{S-2-soln}$	=	the mass of sulfide in the solution [mg]
V_{soln}	=	The volume of the moisture within the mulch [L]
C_{S-2}	=	The concentration of sulfide in the moisture [mg/L]

$$V_{soln} = f_{moist} * M_{mulch} \quad (2)$$

Where,

f_{moist}	=	the fraction of moisture in the sample [g water/g wet mulch]
M_{mulch}	=	the wet mass of mulch used in the test [kg]

The dry mass of the mulch is given by:

$$M_{mulch-dry} = M_{mulch} - (M_{mulch} * f_{moist}) \quad (3)$$

The mass of sulfide from the moisture per mass of mulch is given by:

$$AVS_{soln} = M_{S-2-soln} / M_{mulch} \quad (4)$$

Where,

AVS_{soln}	=	the concentration of AVS due to soil moisture
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Calculation

An example for the Dugway site is as follows:

Given:

C_{S-2}	=	1.045 mg/L
f_{moist}	=	0.1578 (average)
M_{mulch}	=	assume 1 kg

Using (2),

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$$V_{\text{soln}} = 0.1578 * 1 \text{ kg} = 0.1578 \text{ kg} \approx 0.1578 \text{ L}$$

Using (1) yields

$$M_{\text{S-2-soln}} = 1.045 \text{ mg/L} * 0.1578 \text{ L} = 0.165 \text{ mg S}^{-2}$$

Using (3)

$$M_{\text{mulch-dry}} = 1 \text{ kg} - (1 \text{ kg} * 0.1578) = 0.842 \text{ kg}$$

Using (4) yields,

$$AVS_{\text{soln}} = 0.165 \text{ mg} / 0.842 \text{ kg} = \underline{\underline{0.196 \text{ mg/kg}}}$$

mulch dry bulk density =	1.65 g/cc
Mulch porosity =	0.25
TCE Koc =	21 L/kg
foc (SS-17) =	0.0281 wt/wt
Initial TCE Concentration in GW (SS-17) =	3.93 mg/L

PV	Equilibrium Mulch TCE Concentration (mg/kg)	Equilibrium Porewater TCE Concentration (mg/L)	% Adsorbed
1	0.474	0.803	79.6%
2	0.851	1.442	63.3%
3	1.151	1.950	50.4%
4	1.389	2.355	40.1%
5	1.579	2.676	31.9%
6	1.731	2.933	25.4%
7	1.851	3.136	20.2%
8	1.946	3.299	16.1%
9	2.023	3.428	12.8%
10	2.083	3.530	10.2%
11	2.131	3.612	8.1%
12	2.170	3.677	6.4%
13	2.200	3.729	5.1%
14	2.225	3.770	4.1%
15	2.244	3.802	3.2%
16	2.259	3.829	2.6%
17	2.271	3.849	2.1%
18	2.281	3.866	1.6%
19	2.289	3.879	1.3%
20	2.295	3.889	1.04%
21	2.300	3.898	0.82%
22	2.304	3.904	0.66%
23	2.307	3.910	0.52%
24	2.309	3.914	0.41%
25	2.311	3.917	0.33%
26	2.313	3.920	0.26%
27	2.314	3.922	0.21%
28	2.315	3.923	0.17%
29	2.316	3.925	0.13%
30	2.317	3.926	0.11%

Calculation Brief

Objective

To determine the observed TCE degradation rate constant based on decreases in TCE concentrations after passing through the reaction zone.

Methodology

$$k_{\text{overall}} = -\ln(C_{\text{DG}}/C_{\text{UG}})/\zeta \quad (\text{Shen and Wilson, 2007}) \quad (1)$$

where,

k_{overall}	=	The overall rate constant for TCE removal from groundwater [1/hr]
C_{DG}	=	The downgradient (biowall) concentration of TCE [$\mu\text{mole/L}$]
C_{UG}	=	The upgradient concentration of TCE [$\mu\text{mole/L}$]
ζ	=	The residence time of groundwater within the biowall [hrs]

TCE concentrations in $\mu\text{mole/L}$ are calculated from concentrations in $\mu\text{g/L}$ as follows:

$$C (\mu\text{mole/L}) = C (\mu\text{g/L}) / \text{MW}_{\text{TCE}} (\mu\text{g} / \mu\text{mole})$$

Where,

$$\text{MW}_{\text{TCE}} (\mu\text{g} / \mu\text{mole}) = \text{the molecular mass of TCE } (\mu\text{g} / \mu\text{mole} = \text{g/mole})$$

Calculation

An example for the Altus OU-1 site is as follows:

Given:

$C_{\text{DG}} (\mu\text{mole/L})$	=	$550 \mu\text{g/L} / 131.39 \mu\text{g} / \mu\text{mole} = 4.19 \mu\text{mole/L}$
$C_{\text{UG}} (\mu\text{mole/L})$	=	$0.105 \mu\text{g/L} / 131.39 \mu\text{g} / \mu\text{mole} = 0.0008 \mu\text{mole/L}$
ζ	=	13.7 days (measured using a tracer test) = 328.8 hrs

Using (1),

$$k_{\text{overall}} = -\ln(0.0008/4.19)/328.8 = 2.6 \times 10^{-2} / \text{hr}$$

Calculation Brief

Objective

To determine the surface area in m^2/g for a given particle diameter of a mineral.

Methodology

The surface area for a given mineral of a given grain diameter can be determined by making the following assumptions:

- The grains have a cubic morphology (good assumption for pyrite)
- The surfaces of the cubes are smooth (conservative)

The following equations apply:

The surface area of a single cube is given by (as a cube has 6 faces);

$$SA_{\text{Cube}} = 6 * d^2 \quad (1)$$

where,

$$\begin{aligned} d &= \text{The grain diameter (m)} \\ SA_{\text{Cube}} &= \text{The surface area of a single cube of diameter } d \text{ [m}^2\text{]} \end{aligned}$$

The volume of a cube of diameter d is given by;

$$V_{\text{Cube}} = d^3 * (100^3 \text{ cm}^3/\text{m}^3) \quad (2)$$

Where,

$$V_{\text{Cube}} = \text{The volume of a single cube of diameter } d \text{ [cm}^3\text{]}$$

The mass of a single cube of mineral j with density ρ_j is given by;

$$M_{\text{Cube}} = V_{\text{Cube}} * \rho_j \quad (3)$$

Where,

$$\begin{aligned} M_{\text{Cube}} &= \text{The mass of a single cube of diameter } d \text{ [g]} \\ \rho_j &= \text{The density of mineral } j \text{ [g/cm}^3\text{]} \end{aligned}$$

Substituting (2) into (3) yields;

$$M_{\text{Cube}} = d^3 * (100^3 \text{ cm}^3/\text{m}^3) * \rho_j \quad (4)$$

The surface area per mass SA_d for a given grain diameter d is then given by dividing (1) by (4);

$$SA_d = (6 * d^2) / (d^3 * (100^3 \text{ cm}^3/\text{m}^3) * \rho_j)$$

Simplifying yields;

$$SA_d = 6 / (d * (1 \times 10^6 \text{ cm}^3/\text{m}^3) * \rho_j) \quad (5)$$

Calculation

An example for pyrite of grain diameter 8 μm follows:

Given:

$$\begin{aligned} d &= 8 \mu\text{m} = 8 \times 10^{-6} \text{ m} \\ \rho_j &= 5.02 \text{ g/cm}^3 \end{aligned}$$

Using (5) yields

$$SA_d = 6 / (8 \times 10^{-6} \text{ m} * (1 \times 10^6 \text{ cm}^3/\text{m}^3) * 5.02 \text{ g/cm}^3) = \underline{\underline{0.149 \text{ m}^2/\text{g}}}$$

Calculation Brief

Objective

To determine the surface area-normalized rate constant for a given particle diameter.

Methodology

The calculation is performed in the following steps:

1. Calculate the total surface area for each field site using the following:

$$SA_T = SSA_j * C_j \quad (1)$$

Where,

SA_T	=	The total surface area of mineral j [m^2/L]
SSA_j	=	The specific surface area of mineral j of a given particle size [m^2/g]
C_j	=	The concentration of mineral j [g/L]

The concentration of the mineral per Liter of solution (C_j) is determined as follows:

$$C_j = (\rho/n * C_{soil-j})/1000 \text{ mg/g} \quad (2)$$

Where,

ρ	=	The dry bulk density of the mulch [kg/L]
n	=	The total porosity of the mulch [L/L]
C_{soil-j}	=	The concentration of mineral j in the mulch [mg/kg]

In the case of iron monosulfide, C_{FeS} is obtained from the acid-volatile sulfide analysis, which is reported in mg S/kg. Therefore, the mass of FeS/kg mulch (C_{FeS}) would be:

$$C_{FeS} = AVS * (MW_{FeS}/MW_S) * (1 \text{ mole FeS/ mole S}) \quad (3)$$

Where,

AVS	=	The concentration of FeS in the mulch [$mg \text{ S/kg}$]
MW_{FeS}	=	The molecular weight of FeS [$mg/mole$]
MW_S	=	The molecular weight of S [$mg/mole$]

A similar equation is used for iron disulfide (FeS_2) as follows:

$$C_{FeS2} = CrRS * (MW_{FeS2}/MW_S) * (1 \text{ mole FeS}_2/2 \text{ mole S}) \quad (3)$$

Where,

$CrRS$	=	The chromium reducible sulfur [$mg \text{ S/kg}$]
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The total sulfide concentration ($C_{\text{soil-j}}$) would then be:

$$C_{\text{soil-j}} = C_{\text{FeS}_2} + C_{\text{FeS}} \quad (4)$$

Combining 1) through 4) yields:

$$SA_T = SSA_j * (\rho/n * (CrRS * ((MW_{\text{FeS}_2}/MW_S)*(1 \text{ mole FeS}_2/2 \text{ mole S})) + (AVS * (MW_{\text{FeS}}/MW_S)*1)))/1000 \text{ mg/g} \quad (5)$$

2. Determine the ratio of abiotic degradation rate to total surface area for literature values of TCE degradation by iron sulfides.

$$\text{Ratio} = k_{\text{abiotic-experimental}} / SA_{T\text{-experimental}} \quad (6)$$

Where,

$$\begin{aligned} k_{\text{abiotic-experimental}} &= \text{The experimentally determined abiotic degradation rate constant for TCE degradation by FeS [1/hr]} \\ SA_{T\text{-experimental}} &= \text{The total surface area of FeS used in the experiment [m}^2\text{/L]} \end{aligned}$$

The rate constant for a field site with given total surface area SA_T would be given by:

$$k_{\text{field}} = \text{ratio} * SA_T \quad (7)$$

$$k_{\text{field}} = \text{The abiotic rate constant for the field site (1/hr)}$$

Calculation

An example for the Altus OU-1 site is as follows:

Given:

$$\begin{aligned} \rho &= 1.5 \text{ g/cm}^3 \\ n &= 0.42 \text{ (EPA column study)} \\ SSA &= 2 \text{ m}^2\text{/g (value for framboidal pyrite determined by Pugh et al. (1981)} \\ CrRS &= 219 \text{ mg/kg (median value for OU-1)} \\ AVS &= 155 \text{ mg/kg (median value for OU-1)} \\ MW_{\text{FeS}} &= 87,913 \text{ mg/mole} \\ MW_{\text{FeS}_2} &= 119,979 \text{ mg/mole} \\ MW_S &= 32,066 \text{ mg/mole} \\ k_{\text{abiotic-experimental}} &= 5 \times 10^{-4} \text{ /hr (Butler and Hayes, 2001)} \\ SA_{T\text{-experimental}} &= 0.5 \text{ m}^2\text{/L (Butler and Hayes, 2001)} \end{aligned}$$

Using (5) yields

$$SA_T = 2 \text{ m}^2\text{/g} * (1.5 \text{ g/cm}^3/0.42)*((219 \text{ mg/kg}*(119,979/32,066)*1/2)+(155 \text{ mg/kg} * (87,913/32,066)))/1000 \text{ mg/g} = 5.96 \text{ m}^2\text{/L}$$

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Using (6) yields,

$$\text{Ratio} = 5 \times 10^{-4} \text{ /hr} / 0.5 \text{ m}^2/\text{L} = 1 \times 10^{-3} \text{ L/m}^2 \text{ hr}$$

Using (7)

$$k_{\text{field}} = 1 \times 10^{-3} \text{ L/m}^2 \text{ hr} * 5.96 \text{ m}^2/\text{L} = \underline{\underline{5.96 \times 10^{-3} \text{ /hr}}}$$

Appendix F
Carbon Stable Isotope Analysis Data Evaluation

Appendix F

Carbon Stable Isotope Analysis Data Evaluation

Carbon Stable Isotope Analysis Background

When an organic compound is degraded, molecules of the compound that contain the heavier of the two stable isotopes of carbon (^{13}C) are degraded at a slower rate, and tend to accumulate in the residual portion of compound that has not been degraded. This accumulation can be recognized as a shift in the ratio of ^{13}C to ^{12}C in the residual compound. Because the fraction that is ^{13}C is changing, this shift is referred to as isotopic fractionation. The conventional notation for the analysis of the ratio of stable carbon isotopes ($\delta^{13}\text{C}$) does not present the results of the analysis as the ratio of ^{13}C to ^{12}C in the sample. Instead, $\delta^{13}\text{C}$ compares the ratio of ^{13}C to ^{12}C in the sample to the ratio of ^{13}C to ^{12}C in a standard used to calibrate the analytical instrument. If the value of $\delta^{13}\text{C}$ is negative, that means that the ratio of ^{13}C to ^{12}C in the sample is smaller than the ratio of ^{13}C to ^{12}C in the standard. As ^{13}C accumulates in the sample, $\delta^{13}\text{C}$ becomes larger, or less negative.

At any instant in time, $\delta^{13}\text{C}$ in the degradation product that is produced from the reaction will differ from $\delta^{13}\text{C}$ in the parent compound by an amount referred to as the isotopic enrichment factor (ϵ). The value of ϵ is characteristic of a particular compound and a particular reaction. The value of ϵ may be different for biotic and abiotic reactions (Liang et al., 2007). If the reaction mechanism (and its characteristic value of ϵ) is known, then the $\delta^{13}\text{C}$ of the original unfractionated compound and the $\delta^{13}\text{C}$ of the compound after degradation can be used to calculate the extent of degradation:

$$f = e^{(\delta^{13}\text{C}_{\text{groundwater}} - \delta^{13}\text{C}_{\text{source}}) / \epsilon} \quad \text{Equation (1)}$$

Where f is the fraction remaining after degradation, where $\delta^{13}\text{C}_{\text{groundwater}}$ is the isotope ratio in the organic contaminant in the sample of ground water, $\delta^{13}\text{C}_{\text{source}}$ is the isotopic ratio in the unfractionated organic contaminant before degradation has occurred, and (ϵ) is the stable isotope enrichment factor. See section 4.0 of USEPA (2008) [the EPA guide for CSIA] for details.

Due to the uncertainty in the analysis, values for $\delta^{13}\text{C}$ are not considered different unless they vary by more than 1‰, and are not used to estimate degradation unless they differ by 2‰ (Section 4.1.2 of USEPA, 2008).

Values of ϵ for degradation reactions are negative, and the value of $\delta^{13}\text{C}$ in degradation products are more negative than the parent. The $\delta^{13}\text{C}$ in the very first product produced by reaction of a previously unfractionated parent material is equal to the $\delta^{13}\text{C}$ in the parent material plus ϵ (where ϵ is a negative number). As the parent material is degraded, it is fractionated. As a result, the $\delta^{13}\text{C}$ in the parent compound increases, and $\delta^{13}\text{C}$ in the degradation product that is produced at that instant in time also increases concomitantly. As the parent compound is further degraded, the value of $\delta^{13}\text{C}$ in the pool of degraded product increases. When the parent is entirely degraded, the $\delta^{13}\text{C}$ in the pool of degraded product is equal to the $\delta^{13}\text{C}$ in the original undegraded parent compound. See Section 4.5 of USEPA (2008) for further discussion.

This relationship has three important consequences. If the $\delta^{13}\text{C}$ of a degradation product is larger than the $\delta^{13}\text{C}$ of the original parent material, that fact is evidence that the degradation product was further degraded. If an organic compound is entirely degraded and then the first degradation product is further degraded, then the $\delta^{13}\text{C}_{\text{source}}$ for the original parent material is a reasonable upper boundary on $\delta^{13}\text{C}_{\text{source}}$ of the first degradation product using Equation (1). If the first degradation product is not entirely degraded, the $\delta^{13}\text{C}$ in the pool of the first degradation product will be less than $\delta^{13}\text{C}_{\text{source}}$ for the original compound. In this circumstance, the value of $\delta^{13}\text{C}_{\text{source}}$ for the original parent compound will be a conservative upper boundary on $\delta^{13}\text{C}_{\text{source}}$ for the second degradation product. It can be lower (more negative) but not higher. As a result, Equation (1) will produce a conservative lower boundary on the extent of degradation of the second degradation product.

USEPA (2008) provides data for the isotopic enrichment factor (ϵ) for TCE, *cis*-DCE, and *trans*-DCE during anaerobic biological reductive dechlorination. Values for (ϵ) for degradation TCE range from -2.5 to -22.9‰, values for *cis*-DCE range from -14.1‰ to -21.1‰, and values for *trans*-DCE are -21.4‰ and -30.3‰. Liang et al. (2007) provided a value for ϵ for abiotic degradation of TCE on FeS of -33.4‰.

The more negative values produce less change in the value of $\delta^{13}\text{C}$ for the same extent of degradation, and predict less degradation for the same change in the value of $\delta^{13}\text{C}$. The most negative value of ϵ produces the most conservative estimate of the extent of biodegradation in Equation (1).

USEPA (2008) in their Figure 6.1 provide data on the range of $\delta^{13}\text{C}$ that would be expected for TCE that is originally spilled to ground water. The range of values for $\delta^{13}\text{C}$ in TCE sold in commerce is -33.49‰ to -27.80‰. These data were collated to determine a plausible range for $\delta^{13}\text{C}_{\text{source}}$.

Stable Isotopes at Altus AFB

Table F-1 presents the $\delta^{13}\text{C}$ of TCE, *cis*-DCE, *trans*-DCE, and vinyl chloride at the OU-1 site at Altus AFB. The value of $\delta^{13}\text{C}$ in TCE in the up gradient well at the OU-1 site (-25.99‰) is just beyond the high end of the range of $\delta^{13}\text{C}$ in TCE sold in commerce. A value of -25.99‰ will be taken as the best available estimate of $\delta^{13}\text{C}_{\text{source}}$ for TCE at the OU-1 site.

The concentration of TCE up gradient of the OU-1 biowall was 550 µg/L. Although TCE was not detected in the biowall, the concentration thirty feet down gradient of the biowall had “rebounded” to 58 µg/L. Although the removal of TCE in biowall was at least 99.96%, the value for $\delta^{13}\text{C}$ of TCE in the down gradient well (-23.55‰) was almost identical to the value for TCE in the upgradient well (-25.99‰). If -23.55‰ is assigned to $\delta^{13}\text{C}_{\text{groundwater}}$ in Equation (1), and $\delta^{13}\text{C}_{\text{source}}$ for TCE is -25.99‰, and ϵ is the value of Liang et al. (2007) for abiotic degradation (-33.4‰), the fraction remaining is 0.93. At least 7% of the TCE should have degraded, if degradation proceeded through an abiotic reaction with FeS. If the least conservative value for ϵ (-2.5‰) is used in equation (1), the fraction remaining is 0.38. No more than 62% of the TCE originally present in the down gradient ground water could have degraded, under the most favorable conditions, through biological degradation. The value for $\delta^{13}\text{C}$ in TCE in the down

gradient well indicates removal of TCE that is much less than the removal actually attained in the biowall.

Because the TCE that was sampled in the down gradient well had not been extensively fractionated, this indicates that it had not been degraded, and further indicates that it had not passed through the biowall. The pattern of fractionation of stable carbon in the TCE along the flow path indicated that much of the TCE sampled in the down gradient well was already present in the aquifer when the biowall was installed, or had not passed through the biowall as it moved down gradient.

Within the biowall at the OU-1 site, TCE is extensively degraded. The isotopic label in the TCE would be transferred to the DCEs during biological reductive dechlorination, and if there were no further degradation of *cis*-DCE or *trans*-DCE, the value for $\delta^{13}\text{C}$ for *cis*-DCE and *trans*-DCE would be -25.99‰. This value will be used as $\delta^{13}\text{C}_{\text{source}}$ for the DCEs in Equation (1). The values for $\delta^{13}\text{C}_{\text{groundwater}}$ for *cis*-DCE or *trans*-DCE are -0.36‰ and -11.94‰ respectively. Using the most negative value for the isotopic enrichment factors for degradation of TCE to *cis*-DCE or *trans*-DCE, Equation (1) estimates a reduction in concentration of at least 70% for *cis*-DCE and at least 12% for *trans*-DCE.

In the down gradient well, the value for $\delta^{13}\text{C}$ for *cis*-DCE (-22.94‰) is slightly higher than the value for the parent TCE. The most negative value for ϵ predicts that at least 13% of the *cis*-DCE had degraded. The least negative value for ϵ predicts that no more than 19% of the *cis*-DCE had degraded. This is evidence for limited biodegradation of *cis*-DCE, but the isotope data do not make it possible to distinguish degradation in the aquifer down gradient of the biowall from degradation within the biowall.

In the down gradient well, the value for $\delta^{13}\text{C}$ for *trans*-DCE is less than the value for the parent TCE. There is no evidence from the isotope ratios that the *trans*-DCE in water down gradient of the biowall has degraded.

Within the biowall, there was extensive degradation of TCE, *cis*-DCE and *trans*-DCE compared to the concentrations in the up-gradient well. The total concentration of TCE, *cis*-DCE and *trans*-DCE in the up-gradient well was 5.2 $\mu\text{mole/L}$. In the biowall only 0.15 $\mu\text{mole/L}$ remained. These precursors to vinyl chloride were almost entirely degraded, and it is reasonable to use $\delta^{13}\text{C}_{\text{source}}$ for TCE as $\delta^{13}\text{C}_{\text{source}}$ for vinyl chloride. The range of ϵ for anaerobic biological degradation of vinyl chloride provided in USEPA (2008) is -21.5‰ to -31.1‰. Using these values in Equation (1), the $\delta^{13}\text{C}$ of vinyl chloride in the biowall suggests that no less than 36% and no more than 48% of the vinyl chloride was degraded, assuming that vinyl chloride was removed through anaerobic biodegradation.

In the down-gradient well, the value for $\delta^{13}\text{C}$ for vinyl chloride is slightly higher than the value for the parent TCE. Using the published range of values for (ϵ) in Equation (1), between 14% and 19% of the vinyl chloride in the water down gradient of the biowall had degraded. There is evidence for limited degradation of vinyl chloride. As was the case with *cis*-DCE, the isotope data do not make it possible to distinguish degradation in the aquifer down gradient of the biowall from degradation within the biowall.

It is important to note that these calculations of the extent of degradation of DCE and vinyl chloride assume that degradation proceeded through anaerobic biological reductive dechlorination. There are no isotopic enrichment factors available in the literature for aerobic biodegradation of the DCEs or vinyl chloride, or for biodegradation by iron reducing bacteria.

The stable isotope ratios in ground water from the SS-17 site at Altus AFB fall into a similar pattern (**Table F-2**). At the BB04 transect, the up-gradient concentration of TCE was 3,930 µg/L, the concentration in the biowall was 1.45 µg/L, and the concentration in the down gradient well rebounded to 3,150 µg/L. Despite the extensive removal of TCE in the biowall, there was no difference between the $\delta^{13}\text{C}$ for TCE in the up-gradient well and the down-gradient well. This pattern indicates that the TCE in the water sampled in the down-gradient well did not pass through the biowall. The same pattern applies to *cis*-DCE. Concentrations of *cis*-DCE are also reduced in the biowall but rebound in the down-gradient well. The $\delta^{13}\text{C}$ in *cis*-DCE in the up-gradient and down-gradient wells are indistinguishable, indicating that the *cis*-DCE sampled in the down gradient well did not pass through the biowall.

In contrast, the $\delta^{13}\text{C}$ of *cis*-DCE in the biowall at the BB04 transect was higher than the $\delta^{13}\text{C}$ of TCE in the up-gradient well, indicating the *cis*-DCE was being degraded in the biowall. If the $\delta^{13}\text{C}$ of TCE in the up-gradient well is used for $\delta^{13}\text{C}_{\text{source}}$ of *cis*-DCE in Equation (1), the extremes in the values of ϵ for degradation of *cis*-DCE through anaerobic biodegradation predict that from 43% to 56% of the *cis*-DCE in the biowall had been degraded.

The behavior of TCE in the BB05 transect followed the same pattern as in the BB04 transect. The up-gradient concentration of TCE was 154 µg/L, the concentration in the biowall was 2.54 µg/L, and the concentration in the down gradient well rebounded to 376 µg/L. The $\delta^{13}\text{C}$ for TCE in the up-gradient well is -22.00‰, while the $\delta^{13}\text{C}$ for TCE in the down-gradient well is -22.52‰. The values of $\delta^{13}\text{C}$ in TCE agreed with each other within the expected limits of analytical uncertainty. This pattern indicates that the TCE in the water sampled in the down-gradient well did not pass through the biowall. In contrast to the pattern in transect BB05, there was no evidence of degradation of *cis*-DCE in the biowall at transect BB05.

Stable Isotopes at Dover AFB

At the WP-14 biowall demonstration site at Dover AFB, concentrations of TCE were below MCLs except for the down gradient well in the west biowall (**Table F-3**). The $\delta^{13}\text{C}$ in TCE provided no evidence of degradation of TCE in the demonstration sites. Again, the values of $\delta^{13}\text{C}$ in TCE agreed with each other within the expected limits of analytical uncertainty. Concentrations of *cis*-DCE were also low. The maximum concentration of *cis*-DCE (23 µg/L) was encountered in the first (east) biowall.

The $\delta^{13}\text{C}$ in *cis*-DCE in the first biowall was -20.82‰, compared to a value of -25.85‰ for TCE in the up-gradient well at the site, and a value of -23.15‰ for *cis*-DCE in the up-gradient well. Because the $\delta^{13}\text{C}$ in *cis*-DCE in biowall was higher than $\delta^{13}\text{C}$ in plausible sources of *cis*-DCE in the first biowall (TCE or *cis*-DCE in the up gradient well), it is likely that *cis*-DCE was degrading in the first biowall. Similarly, the $\delta^{13}\text{C}$ in *cis*-DCE in second biowall was higher than $\delta^{13}\text{C}$ in plausible sources of *cis*-DCE in the second biowall (TCE or *cis*-DCE between the

biowalls). It is likely that *cis*-DCE was also degrading in the second biowall. As was the case with SS-17 biowall at Altus AFB, there was no evidence of degradation of *cis*-DCE in water down-gradient of the biowalls.

Stable Isotopes at Seneca Army Depot Activity

The behavior of TCE and *cis*-DCE at the Ash Landfill Biowall at Seneca Army Depot Activity, followed a different pattern (**Table F-4**). Concentrations of TCE in groundwater were low (10 µg/L or less), and the values for $\delta^{13}\text{C}$ in TCE varied widely (-36.51‰ to -25.43‰). The lowest values for $\delta^{13}\text{C}$ in TCE occurred in water between the biowalls and down gradient of the second biowall in the flow path. One approach to estimate $\delta^{13}\text{C}_{\text{source}}$ is to select the lowest value at the site. See section 4.2.3.2 of USWPA (2008). If the value of $\delta^{13}\text{C}$ in well TS-MW07 (-36.51‰) represents $\delta^{13}\text{C}_{\text{source}}$ for TCE, then values of $\delta^{13}\text{C}$ for TCE in the biowalls (-25.19‰ in well TS-MW01; -25.43‰ in well TS-MW03; and -27.00‰ in well TS-MW08) indicate removals of 25% to 28% if ϵ is -33.4‰ as reported by Liang et al. (2007) for abiotic transformation. The removals would be 98% to 99% if ϵ is -2.5‰ (the least conservative value for biological degradation complied in USEPA, 2008). Finally, the removals would be from 54% to 59% if ϵ is -12.2‰ (the median value for biological degradation complied in USEPA, 2008). In most of the wells at the site, the concentrations of *cis*-DCE range from slightly higher than concentrations of TCE to more than tenfold higher than concentrations of TCE. The values for $\delta^{13}\text{C}$ of TCE and the concentration distribution of TCE and *cis*-DCE indicate that biodegradation was the most important mechanism for degradation of TCE.

Values for $\delta^{13}\text{C}$ for *cis*-DCE in the biowalls are less than values of $\delta^{13}\text{C}$ for TCE in the same wells, or well up gradient, indicating that *cis*-DCE was further degraded. If the value of $\delta^{13}\text{C}$ for TCE in well TS-MW07 (-36.51‰) represents $\delta^{13}\text{C}_{\text{source}}$ for *cis*-DCE, then values of $\delta^{13}\text{C}$ for *cis*-DCE in the biowalls (-20.82‰ in well TS-MW01; -21.01‰ in well TS-MW03; and -25.89‰ in well TS-MW08) indicate removals of 53% to 67% if ϵ is -14.1‰ (the least conservative value for biological degradation complied in USEPA, 2008), or removals from 40% to 52% if ϵ is -21.1‰ (the most conservative value for biological degradation complied in USEPA, 2008).

Similarly, values for $\delta^{13}\text{C}$ for vinyl chloride in well TS-MW08 and in well TS-MW07 up gradient are less than values of $\delta^{13}\text{C}$ for TCE or *cis*-DCE in the same wells, indicating that vinyl chloride was further degraded. If the value of $\delta^{13}\text{C}$ for TCE in well TS-MW07 (-36.51‰) represents $\delta^{13}\text{C}_{\text{source}}$ for vinyl chloride, then the value of -20.49‰ of $\delta^{13}\text{C}$ for vinyl chloride in well TS-MW08 indicates a removal of 52% if ϵ is -21.5‰ (the least conservative value for biological degradation complied in USEPA, 2008), or a removal of 40% if ϵ is -31.1‰ (the most conservative value for biological degradation complied in USEPA, 2008).

Stable Isotopes at Dugway Proving Grounds

The behavior of TCE and *cis*-DCE at the SWMU-97 Pilot Test at Dugway Proving Grounds followed another pattern altogether (**Table F-5**). With the exception of the injection well, the concentrations of TCE were high (>660 µg/L) and concentrations of *cis*-DCE and vinyl chloride were low (<10 µg/L where detected). Concentrations of TCE, *cis*-DCE and vinyl chloride were low in the injection wells. There is very little accumulation of *cis*-TCE or vinyl chloride in the monitoring wells, indicating that any removal of TCE would be through an abiotic mechanism.

In one of the injection wells (IW02) and in all of the monitoring wells, $\delta^{13}\text{C}$ for TCE ranged from -17.04‰ to -19.71‰. These values are much above any plausible $\delta^{13}\text{C}_{\text{source}}$ for TCE based on known values of $\delta^{13}\text{C}$ in TCE sold in commerce, indicating that TCE had been degraded. In the other injection well, concentrations of TCE were low, but the value of $\delta^{13}\text{C}$ in TCE was -27.99‰, which is very close to the upper end for the range of $\delta^{13}\text{C}$ in TCE sold in commerce (-27.80‰). If a value of -27.80‰ represents $\delta^{13}\text{C}_{\text{source}}$ for TCE, then values of $\delta^{13}\text{C}$ for TCE in the monitoring wells (-17.04‰ to -19.71‰) correspond to removals of 21% to 27% if ϵ is -33.4‰ as reported by Liang et al. (2007) for abiotic transformation. The removals would be 96% to 98% if ϵ is -2.5‰ (the least conservative value for biological degradation compiled in USPEA, 2008). The removals would be 48% to 58% if ϵ is -12.2‰ (the median value for biological degradation compiled in USEPA, 2008).

The values of $\delta^{13}\text{C}$ in *cis*-DCE are much lower than values of $\delta^{13}\text{C}$ in TCE. In most cases, the difference is on the order of -13‰ to -14‰. This is as would be expected if the value of ϵ were typical of biological degradation of TCE to *cis*-DCE by anaerobic biological degradation, and there were no further degradation of the *cis*-DCE.

Reference

US Environmental Protection Agency. 2008. A Guide for Assessing Biodegradation and Source Identification of Organic Ground Water Contaminants using Compound Specific Isotope Analysis (CSIA). EPA 600/R-08/148. December.

Table F-1 - Summary of Carbon Stable Isotope Analysis, OU-1 Biowall Demonstration, Altus AFB, Oklahoma

Sample Identification	Location Description	Analysis (units)	Sample Date	TCE	<i>cis</i>-1,2-DCE	<i>trans</i>-1,2-DCE	VC	Ethene
EPAUMP1	Within Biowall	USEPA Laboratory VOCs (µg/L)	6-Sep-07	550	91.8	3.47	7.7	NA
		VOCs with CSIA (µg/L)	6-Sep-07	1,000	100	6.0	10	0.025
		Carbon Fractionization (‰)	6-Sep-07	-25.99	-27.81	NR	NR	NR
MP1	Within Biowall	USEPA Laboratory VOCs (µg/L)	6-Sep-07	0.21 J	5.27	9.49	53.4	NA
		VOCs with CSIA (µg/L)	6-Sep-07	0.9 J	7.0	20	200	0.32
		Carbon Fractionization (‰)	6-Sep-07	NR	-0.36	-22.21	-11.94	NR
MP4	30' Downgradient	USEPA Laboratory VOCs (µg/L)	6-Sep-07	58.4	186	31.1	82.6	NA
		VOCs with CSIA (µg/L)	6-Sep-07	90	300	60	200	0.69
		Carbon Fractionization (‰)	6-Sep-07	-23.55	-22.94	-29.10	-21.41	NR

Notes:

J - the reported value is an estimated concentration.

NA - not analyzed.

NR - value cannot be calculated due to concentrations less than detection.

µg/L – micrograms per liter.

‰ - parts per thousand or "per mil."

TCE – trichloroethene.

DCE – dichloroethene.

VC - vinyl chloride.

Table F-2 - Summary of Carbon Stable Isotope Analysis, SS-17 Full-Scale Biowall, Altus AFB, Oklahoma

Sample ID	Location Description	Analysis (units)	Sample Date	TCE	cis-1,2-DCE	trans-1,2-DCE	VC	Ethene
BB04U	30' Upgradient	USEPA Laboratory VOCs (µg/L)	6-Sep-07	3,930	79.5	9.53	1.92	NA
		VOCs with CSIA (µg/L)	6-Sep-07	7,000	100	20	4.0 J	0.10
		Carbon Fractionization (‰)	6-Sep-07	-23.68	-22.59	NR	NR	NR
BB04W	Within Biowall	USEPA Laboratory VOCs (µg/L)	6-Sep-07	1.45	2.55	<1.0	0.52	NA
		VOCs with CSIA (µg/L)	6-Sep-07	3.0 J	4.0 J	0.6 J	6.0	0.21
		Carbon Fractionization (‰)	6-Sep-07	NR	-11.95	NR	NR	NR
BB04D	30' Downgradient	USEPA Laboratory VOCs (µg/L)	6-Sep-07	3,150	187	5.98	56.5	NA
		VOCs with CSIA (µg/L)	6-Sep-07	6,000	300	10	100	1.0
		Carbon Fractionization (‰)	6-Sep-07	-23.68	-22.59	NR	NR	NR
BB05U	30' Upgradient	USEPA Laboratory VOCs (µg/L)	6-Sep-07	154	288	12.6	0.88	NA
		VOCs with CSIA (µg/L)	6-Sep-07	300	400	20	2.0 J	0.009 J
		Carbon Fractionization (‰)	6-Sep-07	-22.00	-22.22	NR	NR	NR
BB05W	Within Biowall	USEPA Laboratory VOCs (µg/L)	6-Sep-07	2.54	5.04	0.28 J	1.15	NA
		VOCs with CSIA (µg/L)	6-Sep-07	5.0 J	7.0	0.5 J	2.0 J	0.17
		Carbon Fractionization (‰)	6-Sep-07	NR	-23.68	NR	NR	NR
BB05D	30' Downgradient	USEPA Laboratory VOCs (µg/L)	6-Sep-07	376	79.9	3.31	18.4	NA
		VOCs with CSIA (µg/L)	6-Sep-07	700	90	6.0	40	0.16
		Carbon Fractionization (‰)	6-Sep-07	-22.52	-23.2	NR	-21.36	NR

Notes:

J - the reported value is an estimated concentration.

NA - not analyzed.

NR - value cannot be calculated due to concentrations less than detection.

µg/L – micrograms per liter.

‰ - parts per thousand or "per mil."

TCE – trichloroethene.

DCE – dichloroethene.

VC - vinyl chloride.

Table F-3 - Summary of Carbon Stable Isotope Analysis, Site WP-14 Biowall Demonstration, Dover AFB, Delaware

Sample Location	Location Description	Sample Date	Analysis (units)	Date Analyzed	TCE	cis-1,2-DCE	VC	Ethene
North Transect Monitoring Wells								
TS-MW11	5' Upgradient of East Biowall	3/18/2008	Laboratory VOCs (µg/L)	24-Mar-08	1.7	3.1	<1.0	0.17
			VOCs with CSIA (µg/L)	29-Mar-08	2.0 J	4.0 J	<5.0	0.17
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	30-Jul-08	-25.85	-23.15	NR	NR
TS-MW11D (duplicate)	5' Upgradient of East Biowall	3/18/2008	Laboratory VOCs (µg/L)	24-Mar-08	1.6	3.2	<1.0	0.04
			VOCs with CSIA (µg/L)	29-Mar-08	2.0 J	4.0 J	0.6 J	0.04
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	30-Jul-08	-26.19	-23.56	NR	NR
TS-MW01	Within First (East) Biowall	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	3.8	23	0.064 J	0.078
			VOCs with CSIA (µg/L)	29-Mar-08	1.0 J	9.0	0.8 J	0.078
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	30-Jul-08	-25.88	-20.82	NR	NR
TS-MW02	Between Biowalls	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	1.7	9.6	1.7	0.10
			VOCs with CSIA (µg/L)	29-Mar-08	3.0 J	20	1.0 J	0.10
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	30-Jul-08	-26.22	-26.88	NR	NR
TS-MW03	Within Second (West) Biowall	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	3.1	7.9	<1.0	0.12
			VOCs with CSIA (µg/L)	29-Mar-08	2.0 J	10	2.0 J	0.12
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	30-Jul-08	-25.43	-21.01	NR	NR
TS-MW04	15' Downgradient of West Biowall	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	12	19	12	0.33
			VOCs with CSIA (µg/L)	29-Mar-08	3.0 J	8.0	<5.0	0.33
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	30-Jul-08	-26.08	-24.57	NR	NR

Notes:

J - the reported value is an estimated concentration.

NA - not analyzed.

NR - value cannot be calculated due to concentrations less than detection.

µg/L – micrograms per liter.

‰ - parts per thousand or "per mil."

TCE – trichloroethene.

DCE – dichloroethene.

VC - vinyl chloride.

Table F-4 - Summary of Carbon Stable Isotope Analysis, Ash Landfill Biowall, Seneca Army Depot Activity, New York

Sample Location	Location Description	Sample Date	Analysis (units)	Date Analyzed	TCE	cis-1,2-DCE	VC	Ethene
North Transect Monitoring Wells								
TS-MW11	5' Upgradient of East Biowall	3/18/2008	Laboratory VOCs (µg/L)	24-Mar-08	1.7	3.1	<1.0	0.17
			VOCs with CSIA (µg/L)	29-Mar-08	2.0 J	4.0 J	<5.0	0.17
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-25.85	-23.15	NR	NR
TS-MW11D (duplicate)	5' Upgradient of East Biowall	3/18/2008	Laboratory VOCs (µg/L)	24-Mar-08	1.6	3.2	<1.0	0.04
			VOCs with CSIA (µg/L)	29-Mar-08	2.0 J	4.0 J	0.6 J	0.04
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-26.19	-23.56	NR	NR
TS-MW01	Within First (East) Biowall	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	3.8	23	0.064 J	0.078
			VOCs with CSIA (µg/L)	29-Mar-08	1.0 J	9.0	0.8 J	0.078
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-25.88	-20.82	NR	NR
TS-MW02	Between Biowalls	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	1.7	9.6	1.7	0.10
			VOCs with CSIA (µg/L)	29-Mar-08	3.0 J	20	1.0 J	0.10
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-26.22	-26.88	NR	NR
TS-MW03	Within Second (West) Biowall	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	3.1	7.9	<1.0	0.12
			VOCs with CSIA (µg/L)	29-Mar-08	2.0 J	10	2.0 J	0.12
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-25.43	-21.01	NR	NR
TS-MW04	15' Downgradient of West Biowall	3/19/2008	Laboratory VOCs (µg/L)	24-Mar-08	12	19	12	0.33
			VOCs with CSIA (µg/L)	29-Mar-08	3.0 J	8.0	<5.0	0.33
			Carbon Fractionization- δ ¹³ C (‰)	30-Jul-08	-26.08	-24.57	NR	NR

Notes:

J - the reported value is an estimated concentration.

NA - not analyzed.

NR - value cannot be calculated due to concentrations less than detection.

µg/L – micrograms per liter.

‰ - parts per thousand or "per mil."

TCE – trichloroethene.

DCE – dichloroethene.

VC - vinyl chloride.

Table F-4 - Summary of Carbon Stable Isotope Analysis, Ash Landfill Biowall, Seneca Army Depot Activity, New York (cont.)

Sample Location	Location Description	Sample Date	Analysis (units)	Date Analyzed	TCE	cis-1,2-DCE	VC	Ethene
South Transect Monitoring Wells (Amended with Sulfate)								
TS-MW12	10' Upgradient of East Biowall	3/18/2008	Laboratory VOCs (µg/L)	24-Mar-08	0.29 J	<1.0	<1.0	0.022J
			VOCs with CSIA (µg/L)	29-Mar-08	0.3 J	1.0 J	<5.0	0.022 J
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	30-Jul-08	NR	NR	NR	NR
TS-MW06	Within First (East) Biowall	3/18/2005	Laboratory VOCs (µg/L)	24-Mar-08	0.93 J	1.6	0.88 J	0.12
			VOCs with CSIA (µg/L)	29-Mar-08	<5.0	2.0 J	<5.0	0.12
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	30-Jul-08	NR	NR	NR	NR
TS-MW07	Between Biowalls	3/20/2008	Laboratory VOCs (µg/L)	24-Mar-08	9.8	86	80	0.79
			VOCs with CSIA (µg/L)	3-Apr-08	10	20	20	0.79
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	31-Jul-08	-36.51	-28.55	-25.00	NR
TS-MW08	Within Second (West) Biowall	3/20/2008	Laboratory VOCs (µg/L)	28-Mar-08	10	94	82	2.0
			VOCs with CSIA (µg/L)	3-Apr-08	9.0	80	50	2.0
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	31-Jul-08	-27.00	-25.89	-20.49	NR
TS-MW09	15' Downgradient of West Biowall	3/17/2008	Laboratory VOCs (µg/L)	24-Mar-08	4.5	7.9	<1.0	0.04
			VOCs with CSIA (µg/L)	29-Mar-08	4.0 J	10	4.0 J	0.04
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	30-Jul-08	-33.04	-28.41	NR	NR

Notes:

J - the reported value is an estimated concentration.

NA - not analyzed.

NR - value cannot be calculated due to concentrations less than detection.

µg/L – micrograms per liter.

‰ - parts per thousand or "per mil."

TCE – trichloroethene.

DCE – dichloroethene.

VC - vinyl chloride.

Table F-5 - Summary of Carbon Stable Isotope Analysis, SWMU-97 Pilot Test, Dugway Proving Ground, Utah

Sample Location	Sample Identification	Location Description	Analysis (units)	Sample Date	Date Analyzed	TCE	cis-1,2-DCE	VC	Ethene
TW22	097GW082(TW22)	Downgradient	Laboratory VOCs (µg/L)	24-Apr-08	25-Apr-08	2300	6.1 J	<50	NA
			VOCs with CSIA (µg/L)	24-Apr-08	6-May-08	1,000	3.0 J	<5.0	1.5
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	24-Apr-08	1-Aug-08	-17.87	-31.08	NR	NR
TW22	097FD082(TW22) (Field Duplicate)	Downgradient	Laboratory VOCs (µg/L)	24-Apr-08	25-Apr-08	1300	<50	<50	NA
			VOCs with CSIA (µg/L)	24-Apr-08	6-May-08	1000	3.0 J	<5.0	1.5
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	24-Apr-08	1-Aug-08	-18.10	-30.28	NR	NR
TW23	097GW083(TW23)	Downgradient	Laboratory VOCs (µg/L)	24-Apr-08	25-Apr-08	660	<50	<50	NA
			VOCs with CSIA (µg/L)	24-Apr-08	6-May-08	650	<100	<100	1.3
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	24-Apr-08	1-Aug-08	-17.04	NR	NR	NR
TW24	097GW084(TW24)	Downgradient	Laboratory VOCs (µg/L)	22-Apr-08	23-Apr-08	1300	<20	<20	NA
			VOCs with CSIA (µg/L)	22-Apr-08	2-May-08	1000	<5.0	<5.0	0.44
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	22-Apr-08	31-Jul-08	-18.15	NR	NR	NR
TW25	097GW085(TW25)	Upgradient	Laboratory VOCs (µg/L)	23-Apr-08	25-Apr-08	1400	<50	<50	NA
			VOCs with CSIA (µg/L)	23-Apr-08	2-May-08	1000	0.3 J	<5.0	1.5
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	23-Apr-08	31-Jul-08	-17.86	NR	NR	NR
TW28	097GW088(TW28)	Injection Area	Laboratory VOCs (µg/L)	23-Apr-08	25-Apr-08	1500	<100	<100	NA
			VOCs with CSIA (µg/L)	23-Apr-08	2-May-08	1000	3.0 J	0.7 J	1.4
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	23-Apr-08	1-Aug-08	-17.73	NR	NR	NR

Notes:

J - the reported value is an estimated concentration.

NA - not analyzed.

NR - value cannot be calculated due to concentrations less than detection.

µg/L – micrograms per liter.

‰ - parts per thousand or "per mil."

TCE – trichloroethene.

DCE – dichloroethene.

VC - vinyl chloride.

Table F-5 - Summary of Carbon Stable Isotope Analysis, SWMU-97 Pilot Test, Dugway Proving Ground, Utah (cont.)

Sample Location	Sample Identification	Location Description	Analysis (units)	Sample Date	Date Analyzed	TCE	cis-1,2-DCE	VC	Ethene
TW29	097GW089(TW29)	Down/ Crossgradient	Laboratory VOCs (µg/L)	23-Apr-08	25-Apr-08	1800	<50	<50	NA
			VOCs with CSIA (µg/L)	23-Apr-08	2-May-08	1000	2.0 J	<5.0	1.2
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	23-Apr-08	1-Aug-08	-18.28	-40.49	NR	NR
IW02	097GW090(IW02)	Injection Well	Laboratory VOCs (µg/L)	24-Apr-08	25-Apr-08	<50	<50	<50	NA
			VOCs with CSIA (µg/L)	24-Apr-08	6-May-08	24	3.2 J	<5.0	0.47
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	24-Apr-08	1-Aug-08	-19.71	-55.55	NR	NR
IW03	097GW091(IW03)	Injection Well	Laboratory VOCs (µg/L)	24-Apr-08	25-Apr-08	<20	<20	<20	NA
			VOCs with CSIA (µg/L)	24-Apr-08	6-May-08	7.2	<5.0	<5.0	0.56
			Carbon Fractionization- $\delta^{13}\text{C}$ (‰)	24-Apr-08	1-Aug-08	-27.99	-39.74	NR	NR

Notes:

J - the reported value is an estimated concentration.

NA - not analyzed.

NR - value cannot be calculated due to concentrations less than detection.

µg/L – micrograms per liter.

‰ - parts per thousand or "per mil."

TCE – trichloroethene.

DCE – dichloroethene.

VC - vinyl chloride.